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CRITICAL FLOW

General Theory and Spurious Solutions

by

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Numbers in square brackets refer to viewgraphs.

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Providence, Rhode Island, May 1991

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CRITICAL FLOW

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Part 1. General Theory

It is hardly necessary to emphasize the importance that an accurate prediction of the parameters of critical flow plays in a number of industries, notably in nuclear reactor safety calculations and in metering. In spite of its importance, the literature of the subject still contains erroneous statements. Many of them result from an unjustified belief in the generality of certain conclusions drawn in the elementary study of one-dimensional isentropic flow of a perfect gas with constant specific heats through a convergent-divergent (de Laval) nozzle. This lecture will present a complete and consistent theory of such flows, applicable to any fluid (single- or multiphase) and any channel shape. The study is restricted to the one-dimensional approximation, and, although only adiabatic conditions are discussed, the formalism can be extended to arbitrary conditions at the boundary of the channel.

Elementary Gas Dynamics

We begin by recapitulating the classical results of elementary gas dynamics [5]. The conservation equations in the elementary case can be reduced to a single equation in terms of the Mach number M, the cross-sectional area A and the isentropic index γ. This equation can be integrated explicitly in the form of double-valued function A(M) whose graph is given. All other dependent quantities (T, P, etc.) are expressed in terms of the Mach number alone, as indicated [6]. By the use of a judicious, empirically inspired reasoning, it is possible to sketch a diagram illustrating the variation of M (and hence of P, T, etc.) along the nozzle, given the relation z(A). The set of solutions ("portrait") can be sketched exhibiting the effect of back-pressure, as is well known . The critical point introduces a kind of bifurcation. The critical parameters have fixed values for any γ , and the appearance of shock waves must be treated separately.

[7] In 1953 the speaker with Professor K. Zaremba (dec) introduced the spatial coordinate, z, explicitly and accounted for entropy production by the standard friction coefficient, f. This equation can no longer be integrated explicitly, so a set of graphical solutions [8] was obtained by the method of isoclines. To systematize the study, we performed a topological analysis of the model equation which reveals that certain nozzle shapes could introduce spirals or nodal points, in addition to the standard saddle point. The analysis also clearly showed that the standard critical cross-section (here denoted x*) does not occur at the throat but shifts to the divergent portion. To our further surprise, certain nozzle shapes could lead to the appearance of more than one critical point (here denoted x_1* and x_2*).

The preceding observations lay dormant until the advent of computers emphasized their importance because now the model equation [7] could be programmed to produce numerical solutions, say by employing a Runge-Kutta discretization.

Generalization [9]

Since all mathematical models use the same general algorithm [10], it is reasonable to expect the discovery of features which are common to all models of this class [11]. By way of example, we display the homogeneous equilibrium single fluid, model (H.E.M.). To include relaxation (H.R.M.) we introduce a single relaxation time θ and an evolution equation (32d). These are merely illustrative examples, and we point to the fact that the majority of computer codes in present-day use, including two-fluid models, can be reduced to one, all-purpose form, [12]. To study critical flow it is permissible to simplify to the form of Eqn. (2), rather than using the time-dependent equation, and let the program converge to a steady state (2).

The steady-state model (2) represents a set of n (n=1 or more) ordinary, quasilinear differential equations. In what follows we shall sketch the topological analysis of this matrix equation and so demonstrate its power to obtain an understanding of the underlying physics of the problem without looking for any solutions, analytic or numerical. The unknown, to be determined, state-velocity function is denoted by σ whose variation with z is required.

To discretize the problem [13], we apply Cramer's rule and obtain a set of n simultaneous linear algebraic equations for the local directional vector V which plays a key role in the calculation of the familiar "chains."

Viewgraphs [14] introduces a classification of points in the phase-space Ω formed as a union of σ with z. By contrast, the discretized form [15] introduces a classification of the algebraic equations for V. The difference in these two fundamental understandings leads us to pose the question [16] concerning the presumable lack of congruence between the "portrait" of continuous solutions and the "map" of numerical solutions.

On reflection, one must express surprise that the question has not been emphatically posed in industry (and not only in relation to two-phase flow). The evidently negative answer can have far-reaching consequences.

Topological Analysis [17]

In [18] we show how a trajectory m arises in the phase space when it traces only regular points. When $\Delta = 0$, [19], the vector V becomes normal to z, and the trajectory (m_1 plus m_2) bends over with a maximum at M. Since the flow in a nozzle cannot turn on itself, it is clear that a turning point M can only represent a state at the end of a channel, and since there $\Delta = 0$, choking occurs at the exit cross-section. It is noteworthy that the hypercylinder $\Delta = 0$ divides Ω into a subcritical half-space Ω_1 and a supercritical half-space Ω_2.

Although the illustrations are, of necessity, limited to only two state-velocity variables σ_1 and σ_2, the topological conclusions are valid for any value of n.

The picture in [20] shows the intersection of one of the numerator determinants (say $N_1 = 0$) in the Cramer representation with the hypercylinder $\Delta = 0$ along manifold S. A standard theorem of matrix algebra asserts that all determinants N_i must intersect $\Delta = 0$ along S. Thus, manifold S is the locus of all singular points of our steady-state system (2) from [12].

In the three illustrations [18], [19], [20], we have disregarded degenerate cases which are not likely to occur in real problems.

The topological analysis of system (2) establishes three strong theorems quoted in [21]. The bottom line quotes the characteristic equation for the two nonzero eigenvalues of the linearized matrix $e_{\alpha\beta}$.

The preceding, most remarkable, strong theorems have the effect of showing that even in the most elaborate model, the topological relationships in the neighborhood of a singular point are those of a tangent two-dimensional plane. The explicit conclusion is stated in [22], and [23] illustrates the three typical topological patterns. They are identical with the patterns which occurred in the most elementary case [8]. Viewgraphs [24] and [25] formulate the most important physical conclusions that follow.

The saddle-point pattern shown in [26] clearly resembles the elementary pattern [6]. It emphasizes the fact that the critical pressure ratio P^*/P_0 (P_0– pressure at R) is not a constant; it depends on the equation of state and varies when the nozzle is truncated at different cross-sections in the convergent portion. Most clearly, the critical cross-section does not set-in at the throat but moves downstream.

Part 2. Spurious Solutions [27]

Viewgraphs [28] and [29] recapitulate the contrasting interpretations given to the continuous and discretized version of our problem, first encountered in [14] and [15]. This by itself is an indication, albeit a vague one, that the two methods of solving for a trajectory need not necessarily be identical. Such a suspicion is contrary to the prevailing intuitive conviction that a computer output always represents a correct trajectory. In this lecture we show that the answer to the question posed in [16] is positive in certain regions of the phase space and negative in others.

The thesis becomes clear when we proceed to examine the process of numerically searching for the critical cross-section in a system characterized by a saddle point S [30]. It is recalled that the topological analysis unambiguously specifies two finite directions of vector V at S, denoted V_1 and V_2. It is also recalled that at an infinitely small distance from S the directional vectors are either parallel to P or to z, as shown in the lower insert. Given that a numerical algorithm, based on a grid however small, will never produce a chain which crosses S—the only two in this case which we seek. More precisely, two runs starting with very close boundary conditions at z = 0 will produce either a run of type a(1)-a or b(3)-b. The "map" of such endeavors will give the appearance of a nonconverging code and suggest to the operator futile remedies: (a) a change in the model or (b) a tightening of the computational mesh. The only satisfactory course is to (1) check the character of the singular point, (2) locate the singular point, i.e., the critical cross-section, and (3) determine the directions t_1 and t_2 for V_1 and V_2, and integrate from S outwards. (It is possible to think of alternative schemes, but they all amount to a statement that it is unavoidably necessary to understand the topological structure of the phase space and suitably to supplement the main code, because no numerical code can include a singular point in the trajectory.

Viewgraphs [31] and [32] represent two examples of numerical solutions which contain branches that are clearly either irrelevant or plain wrong. Such branches are called **spurious solutions**; they are also called "ghosts" or "phantoms." Their appearance is rooted in the incorrect handling of a singular point.

In [31] two numerical codes, TRAC-PIA and TRAC-PD2 produce consistent solutions 1_C, which adequately represent the experimental data; they all pass through regular points of the phase space. Whereas a deftly handled code would most probably result in an acceptable

approximation to $2''_E$, the two codes, apparently consistent with each other, result in spurious branches $2''_C$.

A similar interpretation can be put on [33].

The lecture just given fully supports C. Truesdell's admonition [33].

The last viewgraph, [34], lists nine topological studies of various aspects of gas dynamics, which the speaker produced together with his collaborators over a span of nearly forty years.

Note: A more detailed discussion of spurious solutions has been given earlier in the submitted extended abstract, "Spurious Solutions in Critical Two-Phase Flow Numerical Codes."

Part 1. General Theory

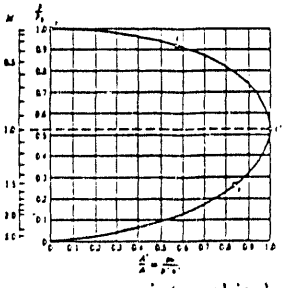
Elementary gas dynamics

Perfect gas with constant specific heats

$$\frac{dM^2}{M^2} = \frac{4(1+kM^2)}{A(z)} \cdot \frac{\gamma f M^2 \cdot A'(z)}{1-M^2} \cdot k = (\gamma-1)/2$$

for isentropic flow (f = 0) this equation can be integrated explicitly with A as independent variable:

$$\left(\frac{A}{A^*}\right)^2 = \frac{1}{M^2} \cdot \left(\frac{1+kM^2}{m}\right)^{m/k} \cdot m = (\gamma+1)/2$$



integral is double-valued

$$T_o/T = 1 + kM^2, \quad P_o/P = (1 + kM^2)^n, \quad n = \gamma/(\gamma-1)$$

etc.

isentropic nozzle flow of perfect gas with constant specific heats

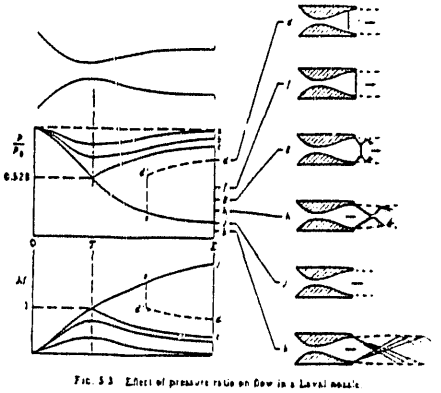


FIG. 5.3 Effect of pressure ratio on flow in a Laval nozzle

Choked isentropic flow

1. Flow is choked when sonic velocity occurs at throat.
2. Pressure ratio P^*/P_0, temperature ratio T^*/T_0 etc. have fixed values.
3. Discontinuous solutions (shock waves) are not described by the differential forms or influence coefficients.

Introduce spatial coordinate z:

$$\frac{dM^2}{dz} = \ldots \frac{\gamma f M^2 \cdot A'(z)}{1-M^2} = \frac{G(M^2,z)}{1-M^2}$$

numerical integration plus topological analysis

singular points at:

$$M^2 = 1, A'(z) = \gamma f \qquad [= 0 \text{ (isentropic)}]$$

$$\text{or } G(M^2, z) = 0$$

singular points in nozzle flows, perfect gas c.s.h.

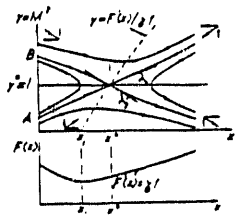
Reprinted from Aircraft Engineering, June 1953

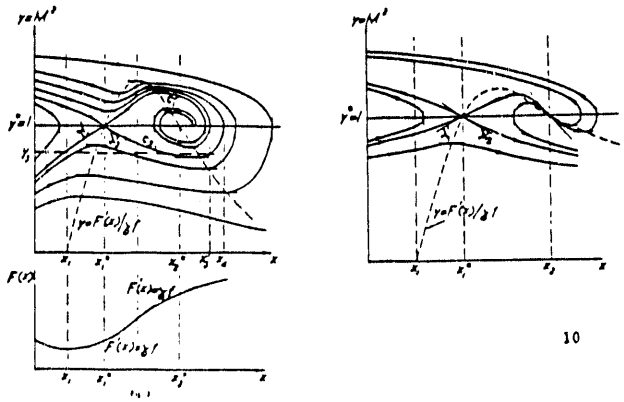
One-Dimensional High-Speed Flows $(F(x) \equiv A(z))$

Flow Patterns Derived for the Flow of Gases Through Nozzles, Including Compressibility and Viscosity Effects

By J. Kestin* and S. K. Zaremba†

Mixed patterns
(Kestin and Zaremba, 1953)





10

Mathematical models

H.E.M. simplest no dispersion

$$D\rho/Dt + \rho\,\partial w/\partial z = -(A'/A)\rho w, \quad (1)$$

$$Dw/Dt + \rho^{-1}\partial P/\partial z = -C\tau/\rho A, \quad (2)$$

$$Dh/Dt - \rho^{-1}DP/Dt = C\tau w/\rho A, \quad (3)$$

$$D/Dt \equiv \partial/\partial t + w\,\partial/\partial z. \qquad \sigma_e = (P, w, h)^T,$$

H.R.M. includes relaxation

$\sigma_e(P, h, w)$ is replaced by $\sigma_n(P, h, x, w)$:

$$D\rho/Dt + \rho\,\partial w/\partial z = -(A'/A)\rho w, \quad (32a)$$

$$Dw/Dt + \rho^{-1}\partial P/\partial z = -C\tau/\rho A, \quad (32b)$$

$$Dh/Dt - \rho^{-1}DP/Dt = C\tau w/\rho A, \quad (32c)$$

$$Dx/Dt = -(x - \bar{x})/\theta, \quad (32d)$$

$$x = \bar{x} - (\bar{x} - x_0)\exp(-t/\theta).$$

Einstein, 1920
Mandel'shtam and Leontovich, 1937
Broer, 1958, 1970

Generalization to any number of phases, arbitrary fluids, and any channel shape

(The "model")

All mathematical models
employ
(single and multiphase flow)
conservation of:
mass
momentum
energy

plus

equations of state
closure conditions

Mathematical model

$$A_{ij}(\sigma)\frac{\partial \sigma_j}{\partial t} + B_{ij}(\sigma)\frac{\partial \sigma_j}{\partial z} = c_i(\sigma, z)$$

$$i, j = 1, \ldots, n$$

$$B_{ij}(\sigma)\frac{d\sigma_j}{dz} = c_i(\sigma, z) \qquad (2)$$

$$\frac{\partial}{\partial t} \equiv 0$$

Set of n ordinary quasilinear differential equations

Topological analysis

(Poincaré, Bendixson, Hale)

Cramer's rule

$$\frac{d\sigma_i}{dz} = \frac{N_i(\sigma,z)}{\Delta(\sigma)}$$

$$V = \frac{d\sigma_i}{dz} = B_{ij}^{-1}\, c$$

$$\sigma(z_{k+1}) = \sigma(z_k) + V_k(z_{k+1} - z_k)$$

(numerical solution - chain)

V_k calculated from
n simultaneous linear
algebraic equations

Continuous solutions:
system of n coupled ordinary nonlinear
differential equations
topological analysis determines
"portrait" in phase space Ω = union $\sigma + z$

classification of points

$\Delta \neq 0$: 1. regular points (σ^o, z^o)
existence and uniqueness
(Cauchy - Kowalewska theorem)

$\Delta = 0$:
2. all $N_i \neq 0$ on $\Delta(\sigma) = 0$
unique trajectory

3. all $N_i = 0$ on $\Delta(\sigma) = 0$
singular points (σ^*, z^*)
nonunique trajectory
topological pattern depends
on nature of singular point

$V = d\sigma / dz = N_i / \Delta$
solution : $\sigma = \sigma(z)$

Discretized solution
system of n coupled linear algebraic equations
solution: chain, e.g., Runge-Kutta
$\sigma_{n+1} = \sigma_n + V_n\,(z_{n+1} - z_n)$
classification of equations

$\Delta \neq 0$: 1. system of equations has
unique solution $\sigma(z)$

$\Delta = 0$:
2. all $N_i \neq 0$, system is
inconsistent, "no solution"

3. all $N_i = 0$, system is
compatible, "infinity" of
solutions

$V_n = (dz/dz)_n = N_{i,n}/\Delta_n$

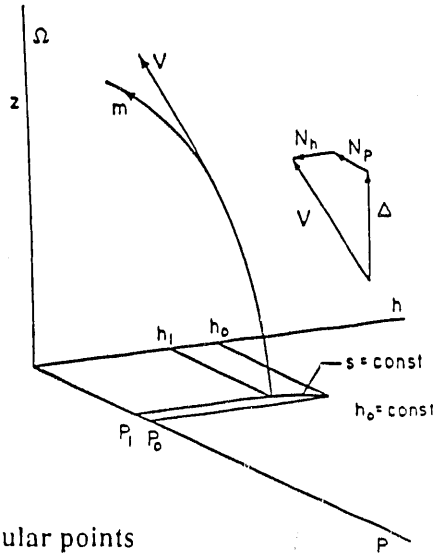
Is the set of trajectories in the phase space

$$\Omega\,(\sigma, z)$$

of model equations the same as the set of system of algebraic equations?

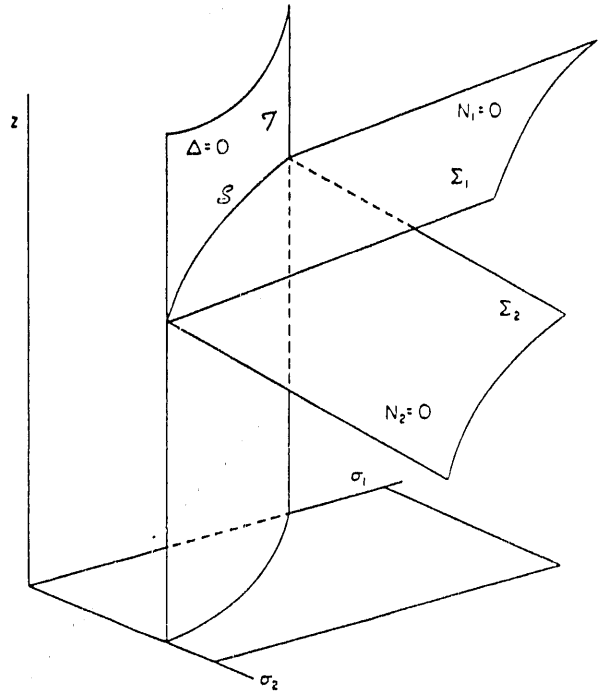
Topological analysis

Trajectory in phase space
V - vector field in Ω
for $\Delta = 0$ V normal to z $(n \neq 0)$

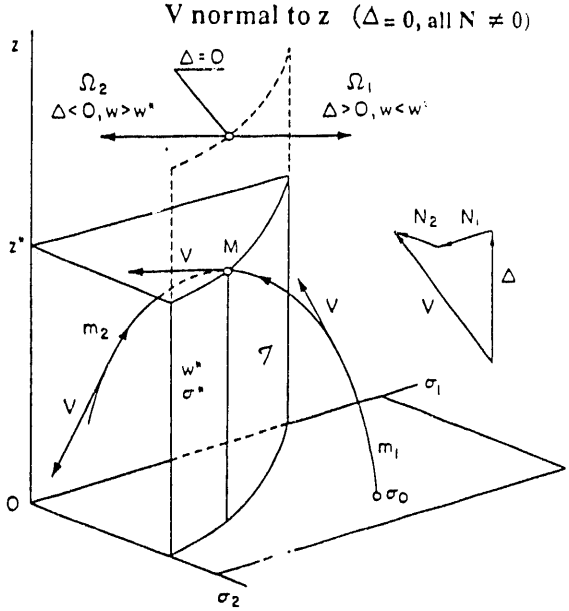


regular points

Singular points
$\Delta = 0$ and all $N = 0$



Turning points (M)
V normal to z $(\Delta = 0, \text{all } N \neq 0)$



choking at end of channel

Topological analysis
(Three strong theorems)

1. All manifolds $N_i = 0$ intersect the manifold $\Delta = 0$ along the same manifold which is thus the locus of all singular (stationary) points of the system.

2. The "phase portrait" in the neighborhood of nondegenerate singular points (rank B_{ij} = n-1, the only relevant case) has the same topology as its linear form.

3. The linearized matrix $e_{\alpha\beta}$ of B_{ij} has only two nonzero eigenvalues.

$$\lambda^2 - \left(\sum_{\alpha=0}^{n} e_{\alpha\alpha}\right)\lambda + \sum_{0\leq\alpha<\beta\leq n}\left(e_{\alpha\alpha}e_{\beta\beta} - e_{\alpha\beta}e_{\beta\alpha}\right) = 0$$

CONCLUSION

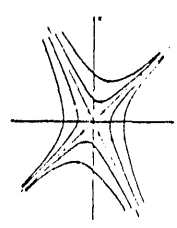
In all present-day
single- and multi-phase
models, it is possible
to encounter only

saddle points
nodal points
spirals

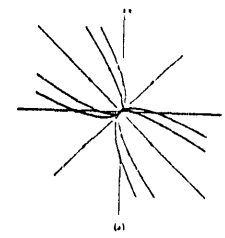
(excepting degenerate cases)

In practice, in convergent-divergent nozzles
(nuclear energy, natural gas meters),
saddle points are most common.

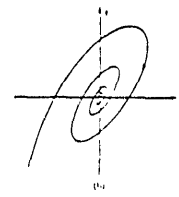
Singular points



saddle point



nodal point



spiral (focus)

Physical conclusions 1

a. Through all points for which $\Delta(\sigma) \neq 0$, called <u>regular</u>, there passes one, and only one, trajectory of system (2) [the Cauchy-Kowalewska theorem].

b. The equation $\Delta(\sigma^*) = 0$ yields the <u>necessary</u> condition for choking which determines the relation between the critical velocity w^* and the remaining state variables. This relation is independent of the channel shape $A(z)$ and the externally controlled closure conditions, all of which are located in the vector c.

c. The conditions

$$\Delta(\sigma^*) = N_i(\sigma^*, z^*) = 0, \qquad (6)$$

with any <u>one</u> N_i, are necessary and sufficient for choking; the value of z^* determines the location $A(z^*)$ of the critical cross-section A^* along a given trajectory. It is clear that z^* is located in the throat of a convergent - divergent nozzle only in isentropic flows of perfect gases. In practice, it is found that A^* places itself in the divergent section of the channel and that relaxation processes drive it quite far downstream from the throat. Mathematically, Equations (6) define a <u>singular point</u> of system (2).

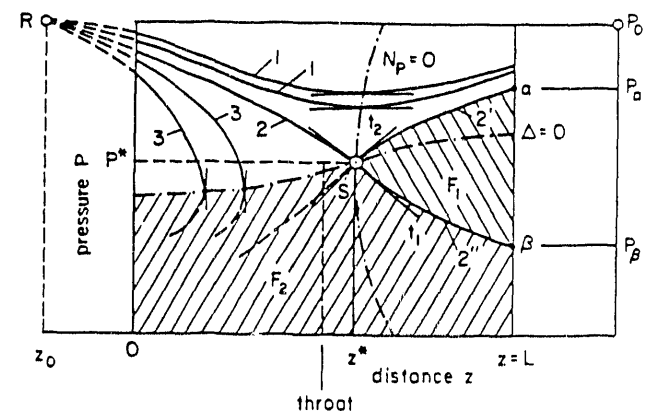
Physical conclusions 2

d. System (2) admits only saddle points, nodal points or spirals, all of which constitute isolated singularities. In practice, in the case of critical two-phase flow, it is sufficient to <u>discuss saddle points</u>.

e. Transition from subcritical ($w<w^*$) to supercritical flow ($w>w^*$) can occur only if the isolated saddle point lies on the respective trajectory.

f. The condition $\Delta(\sigma^*) = 0$, together with $N_i(\sigma^*, z) \neq 0$ [all n components N_i are meant here], can occur only at the end of a convergent or constant-area channel; these are <u>turning points</u>.

Saddle-point pattern
in P, z projection



Part 2. Spurious Solutions

Introduction

A scrutiny of some of the latest critical reviews of the state of the art of modelling thermal-hydraulic phenomena, especially in the context of LWR safety analysis, reveals the persistence of some misconceptions concerning the nature of the flow and of the relation between the preferred mathematical model and its discretized equivalent. It has recently become clear that the ensemble of trajectories in phase space of a mathematical model, expressed in the form of a set of differential equations, can be radically different from the ensemble of solutions implied in the numerical code, expressed as a set of linear algebraic equations employed in practical applications. This discrepancy becomes acute when critical flow rates are computed under conditions of choked flow.

General Mathematical Model

A majority of practical codes make use of the one-dimensional approximation and all of them base it on the standard conservation equations written either as a one-or as a two-fluid formulation. Even though the underlying models differ from each other, they can all be reduced to the following, standard form:

$$A_{ij}(\sigma)\frac{\partial\sigma_j}{\partial t} + B_{ij}(\sigma)\frac{\partial\sigma_j}{\partial z} = c_i(\sigma,z). \qquad (i,j = 1, \ldots, n) \quad (1)$$

Here, σ denotes the vector of dependent state-velocity variables, A_{ij} and B_{ij}, are explicitly known $n \times n$ matrices, though they differ from model to model, as does the vector c_i and the number n of partial differential equations. It should be observed that only the vector c_i contains the coordinate explicitly as it enters the problem through the cross-section profile A(z).

The preceding standard form encompasses the vast majority of computer codes used at present to model single-and multi-phase flows. It is remarkable, as shown by Bilicki and Kestin (1990), that the inclusion of a rate equation (as suggested by Einstein in 1920 and by Mandelshtam and Leontovich in 1937) to account for dispersion and relaxation phenomena fits into the same form and only requires the inclusion of some measure of composition, such as the dryness fraction x, as a component of the state-velocity vector σ.

In order to calculate the critical mass-flow rate, it is possible to allow the code, based on the complete Equation (1), to converge to a steady state. Alternatively, it is possible to base the calculation on the truncated form

$$B_{ij}(\sigma)\frac{d\sigma_j}{dz} = c_i(\sigma,z). \qquad (i,j = 1, \ldots, n) \qquad (2)$$

with

$$\partial/\partial t \equiv 0. \qquad (2a)$$

Although rather obvious intuitively, it can be shown rigorously that the condition of criticality derived by the method of characteristics applied to the set of Equations (1) is completely equivalent to an analysis based on set (2). For this reason we confine our further discussion to an analysis of the truncated Equation (2).

This discretized form is based on the application of Cramer's rule to Equation (2):

$$\frac{d\sigma_i}{dz} = \frac{N_i(\sigma,z)}{\Delta(\sigma)} = B_{ij}^{-1}\, c_j. \qquad (= V) \qquad (3)$$

Here

$$\Delta(\sigma) = \det B_{ij}(\sigma), \qquad (4)$$

and the n determinants $N_i(\sigma,z)$ are obtained from B_{ij} by replacing the j-th column in it by c_j.

Whereas the set (2), presumed adequately to model the

physical situation which is the subject of analysis, constitutes n quasilinear ordinary differential equations, the discretized form (3) can be interpreted as a set of n linear algebraic equations for the components $d\sigma_i/dz$ of directional vectors V. These are then utilized to construct an approximation in the form of the chain

$$\sigma[z_{k+1}] = \sigma(z_k) + V_k\,(z_{k+1} - z_k)\,. \qquad (5)$$

At this point the lecture will pose the question, largely ignored in practically all writings on the subject:

> Is the set of trajectories in the phase space $\Omega(\sigma,z)$ of the Equations (2) the same as the set of chains (5) of the system 3?

The **general** answer, as stated earlier, is in the negative. The ensuing argument will explore the more detailed question concerning the conditions under which the chains (5) are adequate approximations to the trajectories of (2) as well as when the differences between them may give rise to spurious numerical solutions which are either irrelevant or erroneous. The latter case can occur when critical-flow solutions are required.

Topological Properties of General Model

A clear answer to the preceding question is based on a topological analysis of the "portrait" of solutions of system (2) in the phase space $\Omega(\sigma,z)$ contained in Bilicki *et al.* (1987). The theory of dynamic systems establishes the validity of three strong theorems.

1. All manifolds $N_i = 0$ intersect the manifold $\Delta = 0$ along the same manifold which is thus the locus of all **singular (stationary)** points of the system.
2. The "phase portrait" in the neighborhood of nondegenerate singular points (rank B_{ij} = n-1, the only relevant case) has the same topology as its linear form.
3. The linearized matrix $e_{\alpha\beta}$ of B_{ij} has **only two** nonzero eigenvalues.

The preceding rigorously proved propositions lead to the following conclusions.

a. Through all points for which $\Delta(\sigma) \neq 0$, called **regular**, there passes one, and only one, trajectory of system (2) [the Cauchy-Kowalewska theorem].
b. The equation $\Delta(\sigma^*) = 0$ yields the **necessary** condition for choking which determines the relation between the critical velocity w^* and the remaining state variables. This relation is independent of the channel shape A(z) and the externally controlled closure conditions, all of which are located in the vector c.
c. The conditions

$$\Delta(\sigma^*) = N_i(\sigma^*,z^*) = 0, \qquad (6)$$

with any **one** N_i, are necessary and sufficient for choking; the value of z^* determines the location $A(z^*)$ of the critical cross-section A^* along a given trajectory. It is clear that z^* is located in the throat of a convergent - divergent nozzle only in isentropic flows of perfect gases. In practice, it is found that A^* places itself in the divergent section of the channel and that relaxation processes drive it quite far downstream from the throat. Mathematically, Equations (6) define a **singular point** of system (2).
d. System (2) admits only saddle points, nodal points or spirals, all of which constitute isolated singularities. In practice, in the case of critical two-phase flow, it is sufficient to **discuss saddle points**.
e. Transition from subcritical ($w<w^*$) to supercritical flow ($w>w^*$) can occur only if the isolated saddle point lies on the respective trajectory.
f. The condition $\Delta(\sigma^*) = 0$, together with $N_i(\sigma^*,z) \neq 0$ [all n components N_i are meant here], can occur only at the end of a convergent or constant-area channel; these are **turning points.**

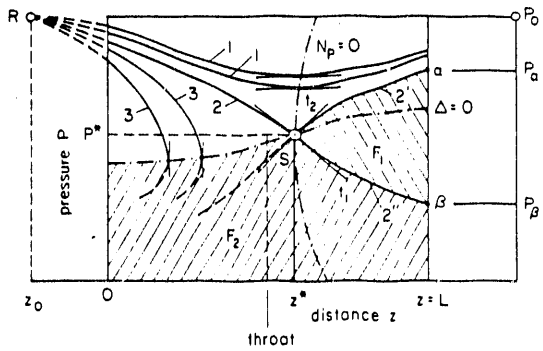


Figure 1. Portrait associated with saddle point. Projection from phase space Ω into P,z plane.

The diagram in Figure 1 depicts the ensemble of solutions ("portrait") in the P,z projection for a convergent - divergent channel when conditions (6) define a saddle point. As already stated earlier, nodal points or spirals, though feasible (*see*, e.g., Kestin and Zaremba, 1953), occur rarely and need not be discussed in this lecture.

The pattern of solutions consists of curves 1, all of which pass through regular points only; such flows are subcritical ($w < w^*$) everywhere. Curves 3 contain turning points along $\Delta = 0$. Clearly, they can occur in a channel only if it is truncated because a physical flow cannot turn on itself in the channel.

Curves 2, 2', and 2" separate the preceding two classes and pass through the saddle point at S where $\Delta = N_P = 0$. The directional vectors t_1, t_2 are determined by the eigenvalues of the linearized matrix $e_{\alpha\beta}$ of B_{ij}. Point S lies on the only trajectories which cross from the subcritical region above $\Delta = 0$ to the supercritical region below $\Delta = 0$.

Curves 2-2" represent critical flow with transition from subcritical to supercritical, whereas curves 2-2' represent choked flow which is fully subcritical, except at S.

The regions denoted by F_1, and F_2 contain trajectories which constitute mathematically correct, but physically unacceptable, solutions of system (2) for flows starting at R.

Discretized Codes

Any numerical code calculates a more-or-less sophisticated version of chain (5) in which $V_k = (d\sigma/dz)$ at z_k results from a matrix inversion of a set of ordinary linear algebraic equations. Such a set has, so-to-say, no knowledge of any singularities. It follows that no numerical code, however advanced, can produce a solution which passes through the saddle point required to determine the critical conditions σ^* or the critical cross-section A^*, and hence the critical mass-flow at choking. It is therefore not surprising that most contemporary algorithms replace their ignorance of conditions (6) by more or less (mostly less) felicitous *ad hoc* assumptions.

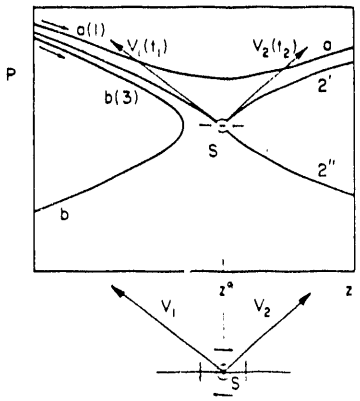


Figure 2. Numerical search for a critical cross-section at z*. Projection from phase space Ω into P,z plane.

To be more explicit, we examine the process of a numerical search for the critical cross-section with the aid of Figure 2. Here S denotes the saddle point in which V_1 and V_2 represent the two tangents t_1, t_2 for Figure 1 whose components can and should be calculated from the linearized matrix $e_{\alpha\beta}$ mentioned above. The two attempts marked a(1) and b(3) start with very close initial conditions and represent the two types of analytic solutions from Figure 1. However, since numerical schemes accumulate errors, the approximations a and b to the trajectories either undershoot or overshoot S, giving the misleading impression of a code which fails the test of convergence. The essential observation is that slopes V_1 and V_2 exist only at S and that those infinitely close are either vertical or horizontal (in this projection), as shown below the diagram. It is, therefore, clear that no forward-marching numerical algorithm will encompass point S and will thus fail to calculate the correct state-velocity components at the critical cross-section or its location z* (different from the throat).

The correct remedy in practical applications is to recognize the inability of a discretized algorithm to produce an approximation to a trajectory which crosses a saddle point. The numerical search with the aid of the main code should be replaced by formulating an **auxiliary code** which locates the saddle point S, Eqns. (6), and integrates in the two explicitly known directions V_1 and V_2. Failure to do so produces spurious solutions. Concrete examples of such misleading answers to important problems will be given in the next section

It should by now be clear that a numerically generated chain, Eqn. (5), is a good approximation to the respective trajectory when the latter passes exclusively through **regular points** at which $\Delta \neq 0$, regardless of the local values of the N_i's, but will fail if the required solution is that which represents choking, that is one which **must** cross the saddle point.

Two Examples of Spurious Solutions

In the open literature there exist no reports of a systematic search for spurious solutions related to two-phase numerical codes. Nevertheless, it is possible to interpret some published data as indicating such evidence.

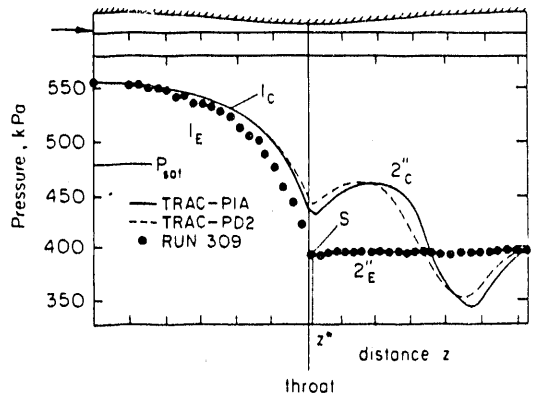


Figure 3. Spurious solution $2''_C$. Measurements and numerical calculations performed at Brookhaven National Laboratory.

The first example, shown in Figure 3, represents a comparison between experimental results of a critical flow of water and steam through a convergent-divergent nozzle and the output of two numerical codes (TRAC-PIA and TRAC-PD2) carried out at Brookhaven National Laboratory (Saha *et al.*, 1982). We assume that the experimental results (circles) represent physical reality and would be reproduced by a successful code. The pattern drawn by the experimental points tracing 1_E and $2_E''$ is consistent with the "portrait" of a saddle point from Figure 1. The putative location of the saddle point, of which the authors do not seem to have taken cognizance, has been placed at z*, somewhat downstream from the throat. The two numerical codes produce results which are consistent with each other along curve 1_C; this is a locus of regular points and contains no spurious solutions. In the absence of a corrective subroutine, both codes produce the spurious solutions denoted $2_C''$, which bear no relation to the physical reality represented by $2_E''$. As expected, the forward-marching codes fail to cross the saddle point, tentatively placed at S. It is noteworthy that both spurious solutions are close, though quite wrong. Further, it is clear that we are not faced here with an unsatisfactory mathematical model or a faulty code. The discrepancy is due to the failure to locate the saddle point.

The second example is a contrived one, though constructed without any thought given to spurious solutions. The diagram represents the output of four standard computer codes of choked flow through identical convergent-divergent nozzles and under identical initial inflow conditions. The exercise, codenamed *Benchmark Test*, was prepared for the International Workshop on Two-Phase Flow Fundamentals (Troy, NY, March 1987, see Hewitt *et al.*, 1991) for the purpose of comparing the consistency of output of these under rigorously controlled conditions. Unexpectedly, certain cases, of which Figure 4 is typical, showed, puzzling at the time, but as presently understood, clear evidence of a spurious solution in the output from IMPI.

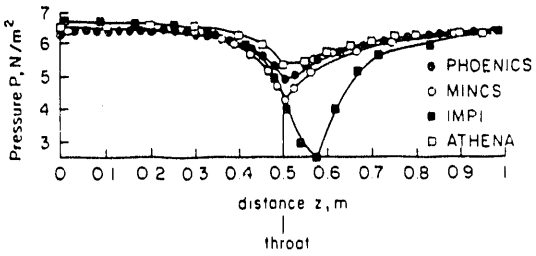


Figure 4. Spurious solution IMPI. Benchmark Test prepared for International Workshop on Two-Phase Flow Fundamentals, 1967.

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