# Studies of Singular Solutions in Dynamic Optimization: I. Theoretical Aspects and Methods of Solution

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For a variational problem in which the control variable is bounded and appears linearly in the system equation, the maximum principle (*11*) seems to indicate an optimal control (optimal operating condition) of the bang-bang type. However, a singular arc may occur when the Hamiltonian function $H$ is not explicitly a function of the control over a finite time interval, and hence the maximum principle does not give adequate information for selecting the optimal control. In this situation, optimal control may actually consist of variable effort, with values intermediate between the upper and lower bounds of the control (called *singular control* on the singular arc). The possible appearance of singular arcs in a problem is usually accompanied by considerable analytic and computational difficulties.

Siebenthal and Aris (*13*) and Paynter and Bankoff (*10*) showed the possible appearance of singular control in the optimal control of a continuous stirred tank reactor and the best design of a tubular reactor. Dyson and Horn (*2*) also indicated that a singular arc occurs in optimal distributed feed reactors. The problem of optimal catalyst distribution along a tubular reactor (*4, 5, 8*) can also be shown to have singular control.

Studies of singular control can be classified into three categories: the definition, characterization, and determination of the existence of singular control; the synthesis of an optimal singular solution; and the derivation of necessary conditions for optimality of the singular arc. Various ways of deriving the necessary conditions for optimality have been studied by several authors (*3, 6, 7*) and will not be discussed here. Construction of the singular surface (*1, 6*) has been very important and useful in characterization and determination of the existence of the singular control. However, each of these authors studied only the free time Bolza problem. For synthesis of the optimal singular solution, most authors (*10, 12*) report using the gradient method. However, the gradient method has the shortcomings of slow convergence, especially close to the optimum, and failure to give a precise optimal control function (*12*). In the present paper, efforts first will be directed to constructing the singular surface for various types of problems and to establishing the criteria for the existence of the singular surface which have not been discussed in the literature. Secondly, a computational algorithm, called the *combined modes method,* developed by the authors, will be presented. It is demonstrated in a companion paper (*9*) that when the new method is used as a terminal refinement scheme with the gradient method, the disadvantages of the latter are largely overcome.

Consider the problem of finding a scalar control function $u(t)$ which maximizes the scalar objective function of Bolza form

$$J = G\,[\mathbf{x}(t_f)] + \int_{t_0}^{t_f} [g_0(\mathbf{x}) + u\, h_0(\mathbf{x})]\, dt \qquad (1)$$

subject to the following conditions:

$$\begin{gathered} \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, u) = \mathbf{g}(\mathbf{x}) + u\, \mathbf{h}(\mathbf{x}), \quad t_0 \leqq t \leqq t_f \\ \mathbf{x}(t_0) = \mathbf{x}_0, \quad u_{\min} \leqq u \leqq u_{\max} \end{gathered} \qquad (2)$$

where $\mathbf{x}$ is an $n$ dimensional state vector and $t_f$ may either be free or fixed. If one defines a Hamiltonian function

$$H(\mathbf{x}, \mathbf{p}, u) = \mathbf{p}^T \mathbf{f} + p_0\, f_0 \qquad (3)^*$$

where $f_0 = g_0(\mathbf{x}) + u\, h_0(\mathbf{x})$, $p_0 = 1$, and an adjoint vector $\mathbf{p}$ by

$$\dot{\mathbf{p}}^T = -\frac{\partial H}{\partial \mathbf{x}} = -p^T(\mathbf{g}_{\mathbf{x}} + \mathbf{h}_{\mathbf{x}}) - (g_{0\mathbf{x}} + f_{0\mathbf{x}}) \qquad (4)$$

with final values prescribed as $\mathbf{p}(t_f) = \partial G/\partial \mathbf{x}(t_f)$, then the maximum principle (*11*) states that the optimal control $\hat{u}(t)$ is chosen so that $H$ is maximized. Furthermore, $\hat{H}$ (maximized $H$) = constant $\geqq 0$. If $t_f$ is free, $\hat{H} = 0$.

If $H$ is written as $H = \psi(\mathbf{x}, \mathbf{p}) + u\, \phi(\mathbf{x}, \mathbf{p})$, then Equations (2) and (3) give

$$\begin{gathered} \phi(\mathbf{x}, \mathbf{p}) = \mathbf{p}^T \mathbf{h}(\mathbf{x}) + h_0(\mathbf{x}) \\ \psi(\mathbf{x}, \mathbf{p}) = \mathbf{p}^T \mathbf{g}(\mathbf{x}) + g_0(\mathbf{x}) \end{gathered} \qquad (5)$$

$H$ is linear with respect to $u$. Accordingly, the optimal control is given by a bang-bang type; that is

$$\hat{u}(t) = \begin{cases} u_{\max} & \text{if } \phi(\mathbf{x}, \mathbf{p}) > 0 \\ u_{\min} & \text{if } \phi(\mathbf{x}, \mathbf{p}) < 0 \end{cases} \qquad (6)$$

If, however, the switching function $\phi$ vanishes identically over a finite time interval, then

$$\phi[\mathbf{x}(t),\ \mathbf{p}(t)] \equiv 0, \quad t_1 \leqq t \leqq t_2 \qquad (7)$$

The Hamiltonian does not explicitly depend on the control $u$, and hence the control law of Equation (6) fails to yield a well-defined optimal control. In this case, an admissible control $u$, which maintains $\phi = 0$ and yields an optimal trajectory, is called a *singular control* (*6, 7*). The corresponding trajectory or subarc is referred as a *singular arc.* Because $\hat{H} = K \geqq 0$, it is to be noted that on a singular arc, $\psi(\mathbf{x}, \mathbf{p}) = K \geqq 0$ and $\psi = 0$, if $t_f$ is free.

## THE SINGULAR SURFACE

The singular surface $S_s(\mathbf{x})$ is the subset of $\mathbf{x}$ at which $\phi$, and all its time derivatives are zero. The singular arc mentioned previously is a part of the singular surface in $\mathbf{x}$ space with added boundaries. The boundaries are determined by the constraint on $u$ (*9*) and the required initial and final conditions for the canonical Equations (2) and (4). The singular surface, in general, is the boundary which sep-

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* $T$ denotes the transpose of a column vector or of a matrix.

arates two different regions of allowable switching direction for bang-bang control (*6*). Knowledge of $S_s$ will then facilitate the analysis and synthesis of the singular solution. Though Johnson (*6*) and Athans and Falb (*1*) have discussed the singular surface and presented methods for constructing it, they limit themselves to the free time problems of Bolza. However, there exist distinctions between free time and fixed time and between the Bolza and Mayer problems in both the characteristics and the criteria for the existence of $S_s$, as well as the methods of construction. The development will first be presented for a two-dimensional case, after which extension to the general $n$ dimensional problem will be briefly discussed.

#### Free Final Time

On the singular arc it is implied that $d^m\phi/dt^m = 0$ for $m = 1, 2, \cdots$. It can be shown that for the problem of Equation (1) (Bolza problem)

$$\frac{d\phi}{dt} = \mathbf{p}^T\,(\mathbf{h}_\mathbf{x}\mathbf{g} - \mathbf{g}_\mathbf{x}\mathbf{h} + h_{0\mathbf{x}}\mathbf{g} - g_{0\mathbf{x}}\mathbf{h}) = 0 \tag{8}$$

or

$$\phi = \mathbf{p}^T\,[\mathbf{q}(\mathbf{x}) + q_0(\mathbf{x})] = 0 \tag{9}$$

where

$$\mathbf{q}(\mathbf{x}) = -\,\mathbf{g}_\mathbf{x}\mathbf{h} + \mathbf{h}_\mathbf{x}\mathbf{g}, \quad q_0(\mathbf{x}) = -\,g_{0\mathbf{x}}\mathbf{h} + h_{0\mathbf{x}}\mathbf{g}$$

Equation (9) together with the equation for $\phi = 0$ [see Equation (5)] are two linear inhomogeneous equations in the adjoint variables, from which $\mathbf{p}$ can be determined:

$$\mathbf{p}(\mathbf{x}) = \mathbf{B}^{-1}(\mathbf{x})\;\mathbf{m}(\mathbf{x})$$

where

$$\begin{aligned}\mathbf{B}(\mathbf{x}) &= [\mathbf{h}(\mathbf{x}):\;\mathbf{q}(\mathbf{x})]^T\\ \mathbf{m}(\mathbf{x}) &= [h_0(\mathbf{x}):\;q_0(\mathbf{x})]^T\end{aligned} \tag{10}$$

It is assumed here that $\det \mathbf{B}(\mathbf{x}) \neq 0$. For a free final time problem on the singular arc, $\psi(\mathbf{x}, \mathbf{p}) = 0$. Substituting Equation (10) into this expression, one obtains the singular surface. Thus

$$S_s : S(\mathbf{x}) = [\mathbf{B}^{-1}\,(\mathbf{x})\;\mathbf{m}\,(\mathbf{x})]^T\mathbf{g}\,(\mathbf{x}) + g_0(\mathbf{x}) = 0 \tag{11}$$

On the other hand, if one finds that $\det \mathbf{B}(\mathbf{x}) = 0$, then one is sure that no singular surface exists and that there is no singular control for this Bolza problem.

If, however, the problem is of Mayer form, that is, $g_0 = h_0 = 0$ in Equation (1), then the criterion is different. If $\det \mathbf{B}(\mathbf{x}) \neq 0$, then Equations (7) and (9) do not have a nontrivial solution for $\mathbf{p}$ and hence there exists no singular surface. But the system may have a nontrivial solution if $\det \mathbf{B}(\mathbf{x}) = 0$, which, of course, must be compatible with the equation $\psi(\mathbf{x}, \mathbf{p}) = 0$. In other words, the solution vector $\mathbf{p} = c\,[b_1(\mathbf{x}),\, b_2(\mathbf{x})]^T$ must be orthogonal to the vector $\mathbf{g}(\mathbf{x})$.

#### Fixed Final Time

If the final time $t_f$ is fixed, then $\psi = K > 0$. Knowledge of $t_f$ introduces an (unknown) constant $K$. This prevents one from determining the singular surface uniquely for the Bolza problem previously described. Following the same procedure used to obtain Equation (11), provided $\det \mathbf{B}(\mathbf{x}) \neq 0$, the expression for the singular surface results:

$$\psi = [\mathbf{B}^{-1}(\mathbf{x})\;\mathbf{m}(\mathbf{x})]^T\,\mathbf{g}(\mathbf{x}) + g_0(\mathbf{x}) = K$$

This equation contains $K$ and defines a one-parameter family of singular surfaces. In general, it is not possible to determine which singular surface corresponds to the one on which the optimal singular arc will stay until the optimal solution is obtained. On the other hand, if $\det \mathbf{B}(\mathbf{x}) = 0$, or the rank of matrix $\mathbf{B}(\mathbf{x})$ is 1, and if the rank of augmented matrix $\mathbf{A}(\mathbf{x}) = [\mathbf{h}(\mathbf{x}):\mathbf{q}(\mathbf{x}):\mathbf{m}(\mathbf{x})]^T$ is greater or equal to 2, then the system [Equations (7) and (9)] does not have a solution. The singular surface does not exist. However, if the objective function is of Mayer form, rather than the Bolza form, then the singular surface can be uniquely determined, if it exists at all.

To recapitulate, the resulting equations are:

$$\begin{aligned}\phi &= h_1(\mathbf{x})p_1 + h_2(\mathbf{x})p_2 = 0\\ \phi &= q_1(\mathbf{x})p_1 + q_2(\mathbf{x})p_2 = 0\end{aligned} \tag{12}$$

The system of Equation (12) has a nontrivial solution for $\mathbf{p}$ if and only if the coefficient matrix vanishes; that is, $\det \mathbf{B}(\mathbf{x}) = 0$, or

$$h_1(\mathbf{x})\;q_2(\mathbf{x}) - h_2(\mathbf{x})\;q_1(\mathbf{x}) = 0 \tag{13}$$

This equation provides a well-defined singular surface $S_s(\mathbf{x})$ without recourse to finding $\mathbf{p} = \mathbf{p}(\mathbf{x})$ first. In fact, the adjoint vector $\mathbf{p}$ on the singular arc cannot be determined until the optimal solution is obtained. The system Equation (12) represents a degenerate system of linear equations. The solution for $\mathbf{p} = \mathbf{p}(\mathbf{x})$ can be obtained up to a real constant $c$, as $\mathbf{p} = c\,[b_1(\mathbf{x}),\, b_2(\mathbf{x})]^T$. The constant $c$ is implicitly defined by $\psi(\mathbf{x}, \mathbf{p}) = K$.

The above approach and theory can be extended to the general $n$ dimensional problem if $(n-1)$ repeated differentiations of the switching function do not contain $u$ explicitly. In such cases, for a free time problem of Bolza, the adjoint vector $\mathbf{p}$ which belongs to the singular integral manifold $R_s(\mathbf{x}, \mathbf{p})$ (*6*), can be solved in terms of the state vector $\mathbf{x}$. The resulting expression $\mathbf{p}(\mathbf{x})$ can then be substituted into the function $\psi(\mathbf{x}, \mathbf{p}) = 0$ to determine uniquely the singular surface. For a problem of fixed final time with an objective function of the Mayer form, $\mathbf{p} \in R_s\,(\mathbf{x}, \mathbf{p})$ cannot be determined explicitly in terms of $\mathbf{x}$. However, $S_s(\mathbf{x})$ can be constructed uniquely from the singular condition of the coefficient matrix of $\mathbf{p}$. For a fixed time but a Bolza form objective function, $S_s$ can be determined up to a constant parameter.

In general it is likely that the control $u$ will appear explicitly before the $(n-1)^{\text{th}}$ differentiation for $n \geqq 3$. If it does so, the singular surface cannot be determined, except for a linear system with a quadratic objective function (*14*). In such a situation, it will probably be easier to consider both $\mathbf{x}$ and $\mathbf{p}$ spaces (*8*).

If $S_s$ can be defined in $\mathbf{x}$ space, then the singular control $u_s$ can be derived in terms of $\mathbf{x}$ only. Thus

$$\frac{d}{dt}\,S(\mathbf{x}) = S_\mathbf{x}\;[\mathbf{g}(\mathbf{x}) + \mathbf{h}(\mathbf{x})\cdot u] = 0$$

from which $u_s$ can be obtained as $u_s(\mathbf{x}) = -\,S_\mathbf{x}\mathbf{g}(\mathbf{x})/S_\mathbf{x}\mathbf{h}(\mathbf{x})$. The control in this expression is, of course, also subject to the constraint $u_{\min} \leqq u_s(\mathbf{x}) \leqq u_{\max}$. If $S_\mathbf{x}\mathbf{h}$ vanishes identically, then a repeated time differentiation should be taken until one obtains an expression which contains $u(t)$ explicitly. Knowledge of $u_s(\mathbf{x})$ provides valuable information regarding the synthesis of optimal singular control.

### METHODS OF SOLUTION

The previous discussion has been limited to definitions, characterization of singular problems, and the construction of the singular surface. In this section a more important question, the methods of obtaining an optimal control function which consists of both singular control and bang-bang control, will be considered.

#### Method of Gradient

The gradient method is well known, and a large number of publications have been concerned with its application to the problems of nonsingularity. Recently, Paynter and Bankoff (*10*) and Sienfeld and Lapidus (*12*) have experienced some success in applying the method to find the optimal singular solution. The gradient method can be shown (*8*) feasible for obtaining the singular solution, since in the derivation of the algorithim the maximum principle has not been applied, and the form of $u(t)$ has not been assumed. Yet, the algorithm sequentially improves the objective function. However, results indicate (*9, 10, 12*) that the method appears to give a very slow convergence close to the optimum and cannot provide a precise form of the optimal control function. To overcome these difficulties, the combined modes method has been developed to serve as a terminal refinement scheme.

**Combined Modes Method**

One shortcoming of a gradient process is that over intervals on which $\partial H/\partial u$ is small in magnitude, the corresponding changes in $u(t)$ will also be small. After several steps $u(t)$ may still be far from the optimal values over such insensitive intervals. This is particularly true for a singular problem in which $\partial H/\partial u$ vanishes identically on a singular arc. Recall that $H = \psi + u\,\phi$. On the singular arc, $\phi = 0$, and on the bang-bang arc, the optimal control $u(t)$ either assumes the upper bound $u_{\max}$ or the lower bound $u_{\min}$ for either of which $\phi \neq 0$. This indicates that on the bang-bang portion, the value of $|\phi(\mathbf{x}, \mathbf{p})|$ will be considerably greater than that on the singular arc, especially when the successive approximation procedure proceeds closer to the optimum.

At the bang-bang switching point $t_b$, the switching function has isolated zeros. That is

$$\phi[x(t),\ p(t)] \approx 0, \quad t_b - \Delta t < t < t_b + \Delta t$$

during the process of successive approximation, where $\Delta t \rightarrow 0$ when the optimum is reached. In order to identify the singular arc, one needs further information. Equation (8) shows that $d\phi/dt$ does not explicitly contain the control and vanishes identically on the singular arc. However, it can be shown that during the sequential time differentiation of $\phi$, a function in which the control variable appears explicitly can be obtained. That is

$$\frac{d^k}{dt^k}\,\phi(\mathbf{x}, \mathbf{p}) = \beta(\mathbf{x}, \mathbf{p}) + u\,\gamma(\mathbf{x}, \mathbf{p}) = 0$$

where $\gamma(\mathbf{x}, \mathbf{p}) \neq 0$, $k \geqq 2$. Solving the above equation for $u(t)$, one obtains

$$u_s\,(\mathbf{x}, \mathbf{p}) = -\frac{\beta(\mathbf{x}, \mathbf{p})}{\gamma(\mathbf{x}, \mathbf{p})} \tag{14}$$

This is the control which has to be maintained on the singular arc.

In adopting the control $u(t) = u_s(t)$ generated by Equation (14) as the next approximation, one violates the linearization assumption, for this may represent a large step process. More conservatively, one may choose to replace the large step by an exploratory series of small ones, setting

$$u^{i+1}(t) = u^i(t) + \eta\,[u_s{}^i(t) - u^i(t)], \quad t_1 \leqq t \leqq t_2 \tag{15}$$

where $(t_1, t_2)$ is a singular interval and $\eta$ is a small positive constant such that $0 < \eta < 1$. (Superscript $i$ stands for the $i^{\text{th}}$ iteration.) Since, in general, singular control assumes an intermediate value between the upper and lower bounds of the control variable, when $u^i(t)$ is either at the upper or the lower bound of $u(t)$, the control iteration should follow the gradient method of handling the control on the constraints. In summary, the following control iteration scheme is proposed.

1. If $u^i$ is an interior point of the control constraint, that is $u_{\min} < u^i(t) < u_{\max}$ then

$$\delta u^i = u^{i+1} - u^i = \eta\,(u_s{}^i - u^i), \quad \text{if}$$

$$|\phi^i(\mathbf{x}, \mathbf{p})| < \epsilon', \quad |\dot{\phi}^i| < \epsilon'' \tag{16}$$

$$\text{and if } u_{\min} < u_s{}^i(t) < u_{\max}$$

and

$$\delta u^i = \epsilon\left(\frac{\partial H}{\partial u}\right)^i, \ \text{otherwise}\ (\epsilon > 0) \tag{17}$$

2. If $u^i$ is on the constraint of the control at the upper limit, $u^i(t) = u_{\max}$

$$\begin{aligned} \delta u^i &= \epsilon\left(\frac{\partial H}{\partial u}\right)^i, \ \text{if}\ \left(\frac{\partial H}{\partial u}\right)^i \leqq 0 \quad (\epsilon > 0) \\ \delta u^i &= 0, \qquad \text{if}\ \left(\frac{\partial H}{\partial u}\right)^i \geqq 0 \end{aligned} \tag{18}$$

at the lower limit, $u^i(t) = u_{\min}$.

$$\begin{aligned} \delta u^i &= \epsilon\left(\frac{\partial H}{\partial u}\right)^i, \ \text{if}\ \left(\frac{\partial H}{\partial u}\right)^i \geqq 0 \quad (\epsilon > 0) \\ \delta u^i &= 0, \qquad \text{if}\ \left(\frac{\partial H}{\partial u}\right)^i \leqq 0 \end{aligned} \tag{19}$$

In Equation (16), $u_s(t)$ is, of course, also subject to the constraint. That is, if $u_s$ is outside the bounds, then the gradient mode [Equation (17)] should be used. Determination of the small positive constants $\epsilon$, $\epsilon'$, $\epsilon''$ becomes relatively easy after the iteration procedure has progressed and before we switch to the combined modes method.

There is, of course, a question of convergence with the scheme given in Equations (16) through (19). To answer this question one might proceed to the following analysis.

Maximizing $J$ is equivalent to maximizing $L$ (a Lagrangian) for a successive approximation procedure

$$L = G\,[\mathbf{x}(t_f)] + \int_{t_0}^{t_f} [f_0 + \mathbf{p}^T\,(\mathbf{f} - \dot{\mathbf{x}})]\,dt$$

in which $\mathbf{f} - \dot{\mathbf{x}} = 0$ is satisfied identically in each iteration. The variation of $L$ from the $i^{\text{th}}$ to the $(i+1)^{\text{th}}$ iteration can be shown to be

$$\begin{aligned} \delta L = L^{i+1} - L^i &= \int_{t_0}^{t_f} [H(\mathbf{x}^i, \mathbf{p}^i, u^i + \delta u^i) \\ &\quad - H(\mathbf{x}^i, \mathbf{p}^i, u^i)]\,dt = \int_{t_0}^{t_{1-}} \left(\frac{\partial H}{\partial u}\right) \delta u^i\,dt \\ &\quad + \int_{t_{1+}}^{t_{2-}} [H(\mathbf{x}^i, \mathbf{p}^i, u^i + \delta u^i) - H(\mathbf{x}^i, \mathbf{p}^i, u^i)\,dt \\ &\quad + \int_{t_{2+}}^{t_f} \left(\frac{\partial H}{\partial u}\right)^i \delta u^i\,dt \end{aligned} \tag{20}$$

Convergence of the first and third integrals on the bang-bang portion is obtained if $\delta u^i$ follows the gradient method (8). Hence the convergence of $L$ depends on whether or not the increment $\delta L'$ is positive:

$$\delta L' = \int_{t_{1+}}^{t_2} [H(\mathbf{x}^i, \mathbf{p}^i, u^i + \delta u^i) - H(\mathbf{x}^i, \mathbf{p}^i, u^i)]\,dt$$

Evidently, a sufficient condition for $\delta L' > 0$ for small $\eta$ is

$$\lim_{\eta \to 0}\ [H(u^i + \eta\,(u_s{}^i - u^i)) - H(u^i)]$$

$$= \left(\frac{\partial H}{\partial u}\right)^i \eta(u_s^i - u^i) > 0, \quad t_1 < t < t_2 \quad (21)$$

which requires that the directional derivative of $H^i$ be positive in the direction of the singular control point $u^i = u_s^i(t)$. The authors are not able to derive Equation (21) in a rigorous fashion. However, the requirement of Equation (21) will probably be met globally if the objective function possesses no stationary points or extrema in the region $u_{min} < u < u_{max}$ other than the maximum $u^i(t) = u_s^i(t)$. In other words, if the optimal solution contains the singular arc, then the equation should hold in the interval $(t_1, t_2)$. Furthermore, if the combined modes solution is used as a terminal refinement scheme of successive approximation, only a local version of the requirement of Equation (21) needs consideration. In this case, the requirement should be met if the gradient process has progressed well before transition to the combined modes scheme.

In the experience obtained in the examples given in the companion paper (*9*) and in reference *8*, it appears that the combined modes solution procedure converges to a solution which is a better approximation to the optimal solution than normally obtainable with a gradient method, as far as details of the optimal control time history $u(t)$ are concerned. Furthermore, it gives a faster convergence than the gradient method, when it is used as a terminal refinement scheme.

## NOTATION

$\mathbf{B}(\mathbf{x})$ = coefficient matrix
$\mathbf{f}(\mathbf{x}, u)$ = vector state equation
$\mathbf{g}(\mathbf{x})$ = vector function in state equation
$g_0(\mathbf{x})$ = scalar function in the objective function
$G[\mathbf{x}(t_f)]$ = term in the objective function
$\mathbf{h}(\mathbf{x})$ = vector function in the state equation
$h_0(\mathbf{x})$ = scalar function in the objective function
$H$ = Hamiltonian function
$J$ = objective function
$K$ = a positive constant
$L$ = Lagrangian function
$\mathbf{m}(\mathbf{x})$ = matrix
$\mathbf{p}$ = adjoint vector
$\mathbf{q}(\mathbf{x})$ = vector function in Equation (9)
$S_s$ = singular surface
$t$ = time or other independent variable
$u$ = control variable
$u_s$ = singular control
$\mathbf{x}$ = state vector
$\beta, \gamma$ = scalar functions in Equation (14)
$\epsilon, \epsilon' \epsilon''$ = small positive constants
$\eta$ = small positive constant
$\phi(\mathbf{x}, \mathbf{p})$ = switching function
$\psi(\mathbf{x}, \mathbf{p})$ = scalar function in the Hamiltonian function

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# Bubble Coalescence in Fluidized Beds: Comparison of Two Theories


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Lin (*1*) presented an analysis of the motion of a pair of two-dimensional bubbles in vertical alignment based on Murray's (*3*) approximate equations for continuum flow of gas and particles in fluidized beds. Since these equations describe steady flow, the analysis is restricted to situations in which there is no relative motion between the bubbles. Therefore, Lin predicted the separation at which two bubbles have exactly the same velocity, assuming that the bubbles are exactly circular. He obtained the velocity potential describing particle flow relative to the bubbles and inserted this velocity potential into Murray's equations of motion to give an equation for the gas pressure. The condition that the gas pressure should be constant over the surface of each bubble in the vicinity of the nose then led to two independent equations, which were solved numerically to give the stable bubble spacing and rise velocity. The numerical predictions are shown in in Figures 1 and 2.

Clift and Grace (*2*) analyzed the motion of a bubble through a complex flow field resulting from any number of interacting bubbles in a fluidized bed. The analysis was based on Jackson's equations of motion (*4*), and it covered unsteady flow situations, since the effect of relative bubble motion on pressure was included (although smaller effects due to bubble acceleration were neglected). Each bubble was represented by a single doublet so that the resulting bubble boundaries were not exactly circular. It was shown that the velocity of a bubble in a fluidized bed may be approximated by adding its rise velocity in isolation to the velocity which the particulate phase would have at the position of the nose if the bubble were absent.

## QUANTITATIVE COMPARISON

The theory of Clift and Grace covers unsteady motion of interacting bubbles in any orientation. If the distance between the centers of two bubbles in vertical alignment is $d$, then the theory predicts (*2*) that the relative velocity between the bubbles vanishes when

$$1 + \frac{s^{2.5}}{(D+1)^2} = s^{0.5} + \frac{1}{(D-s)^2} \quad (1)$$

where the bubble radii are, respectively, $r_1$ and $r_2$, $s$ is the size ratio $(r_2/r_1)$, and $D$ is the dimensionless separation $(d/r_1)$. Equation (1) defines a relationship between