# Stability of Moving Surfaces in Fluid Systems with Heat and Mass Transport

## III. Stability of Displacement Fronts in Porous Media

Two effects not considered in previous work can significantly influence stability of moving displacement fronts in porous media. They are transport near the front and expansion or contraction accompanying phase change or chemical reaction at the front. It is shown that both effects act to stabilize a moving front at which steam condenses and displaces water. Available experimental data confirm that such a front is more stable than would be expected based on previous work. The effects should be important in steam drive and underground combustion processes for improving oil recovery and in processes involving moving reaction fronts in packed beds.

**CLARENCE A. MILLER**

Department of Chemical Engineering
Carnegie-Mellon University
Pittsburgh, Pennsylvania 15213

## SCOPE

Existing technology for recovery of oil from underground reservoirs typically involves (1) recovery from individual wells using pumps as needed to supplement natural driving forces such as reservoir gas pressure and (2) injection of water into some wells to drive oil to other wells where it can be recovered. Even in reservoirs where this water flooding process is successful, however—generally speaking, those containing oils of relatively low viscosity—about 50 to 60% of the oil originally present remains in the ground after water flooding. This residual oil exists primarily as drops or globules trapped in the small pores of the reservoir rock. For reservoirs with rather viscous oils, water flooding is not attractive and an even greater percentage of the oil is not recovered. Strong incentives obviously exist to improve recovery capabilities.

One class of improved processes, the thermal class, was originally developed for reservoirs with viscous oils. The idea was that heat would reduce oil viscosity and facilitate recovery. But because heat can vaporize trapped oil drops, these processes are also possibilities for getting additional oil from reservoirs which have been water-flooded. The heat is supplied either by injecting steam or by injecting air to burn a small fraction of the oil. In the former case, a front at which steam condenses moves through the reservoir. In the latter case, there is a moving combustion front. In both cases, stability of the moving front between injected and displaced fluids is crucial. For, if instability occurs, the injected fluids contact only a small portion of the reservoir and effectiveness of the process is greatly limited.

Previous work on stability of displacement fronts in porous media has concentrated on effects of fluid viscosity and medium permeability. In this paper, two other effects likely to be important for the processes described above are also considered. One is a heat transport effect analogous to the transport effect responsible for dendrite formation and related instabilities during solidification processes. The other effect is expansion or contraction accompanying a phase change such as condensation or a chemical reaction such as combustion at a moving displacement front. This effect is known to significantly influence flame stability during ordinary combustion processes.

## CONCLUSIONS AND SIGNIFICANCE

A small-amplitude stability analysis of a moving displacement front at which steam condenses shows that both heat transport and the decrease in volume accompanying condensation have significant stabilizing influences. They can sometimes overcome the relatively large destabilizing effect associated with displacing one fluid (water) by a much less viscous fluid (steam), a prediction which is in accord with available experimental data. Heat transport is particularly effective in stabilizing disturbances with short wavelengths so that in cases where instability does occur, the unstable wavelengths may be quite long.

These results provide new insight about the basic mechanism of front stability in porous media. They demonstrate that the well-known effects of fluid viscosity and medium permeability are not the only important influences on front stability—at least when significant temperature or concentration gradients exist or significant volume changes due to phase transformation or chemical reaction occur. This conclusion is of interest in connection with thermal processes for oil recovery, for example, steam drive and underground combustion. But applications may also exist for processes where there are moving reaction fronts in packed beds and for certain underground processes for gasifying coal or retorting oil shale.

The first two papers in this series (Miller and Jain, 1973; Miller, 1973) examined stability of fluid interfaces moving as a result of phase transformation or mass transfer. A simple example of such motion is that accompanying the continuous decrease in size of an evaporating drop.

Here a similar approach is used to investigate stability of moving displacement fronts in porous media. Previous work (Saffman and Taylor, 1958) has shown that fluid mechanical effects have an important influence on stability of such fronts. Instability occurs when a fluid of high mobility (ratio of effective permeability to fluid viscosity) displaces a fluid of low mobility. For the simple case where permeability is uniform throughout the medium, an unstable front exists when a fluid of low viscosity displaces one of high viscosity. For this reason, water flooding is largely ineffective as a means of recovering high viscosity crude oils from underground reservoirs. In addition to this viscosity effect, the present work considers effects of heat transport and of change in volume experienced by fluid crossing the front as it reacts or changes phase. As indicated above, these effects have not previously been considered for situations involving porous media, but they are known to be important in other applications.

A detailed analysis is presented below for stability of a moving front at which steam condenses. This simple case has been chosen to illustrate clearly the basic physical effects involved. A numerical example is given and implications of the results for steam drive and underground combustion oil recovery processes are briefly discussed.

## FLAT CONDENSATION FRONT

Figure 1 illustrates a situation where steam condenses and displaces water in a porous medium along a flat displacement front moving at velocity $V$. Superficial fluid velocity $V_i$, density $\rho_i$, viscosity $\mu_i$, and other fluid properties are taken as uniform in each phase. Steam temperature is presumed to be uniform at the saturation temperature $T_1$ corresponding to mean reservoir pressure. Water temperature varies from $T_1$ at the condensation front to ambient reservoir temperature $T_{2\infty}$ at large distances from the front.

For small fluid velocities, as are generally encountered in oil reservoirs, Darcy's Law applies, so that in a stationary coordinate system

$$V_i = -\frac{k_i}{\mu_i}\frac{\partial}{\partial Z}(P_i - \rho_i g_Z Z) = \frac{\partial \Phi_i}{\partial Z} \qquad (1)$$

Here $k_i$, $P_i$, and $\Phi_i$ are reservoir permeability, fluid pressure, and velocity potential in phase $i$ and $g_Z$ is the component in the direction of flow of the acceleration due to

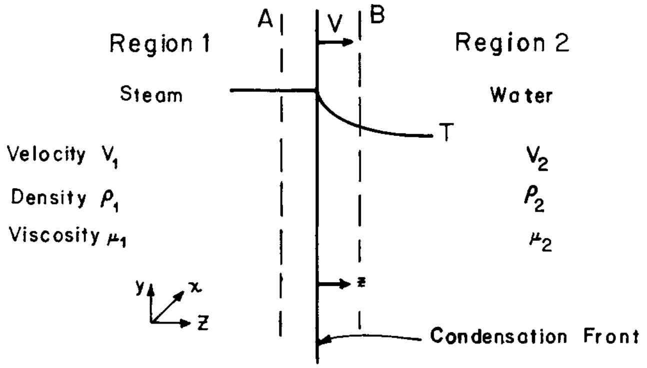


**Fig. 1. Moving front at which steam condenses and displaces water in a porous medium.**

gravity. A mass balance for the stationary control volume between lines A and B of Figure 1 yields the following result:

$$\rho_1 V_1 - \rho_2 V_2 = \epsilon V(\rho_1 - \rho_2) \qquad (2)$$

In this equation, $\epsilon$ is reservoir porosity.

It should be noted that the assumption of one-dimensional flow implicit in (1) and (2) is not truly correct except when flow is vertical. For otherwise, gravity causes steam to rise and flow preferentially in the upper part of the medium with a corresponding preferential flow of water in the lower part of the medium. For simplicity this gravity override effect is neglected here as the main purpose is to illustrate transport and volume change effects on stability. In actuality, both gravity override and stability may be important, and an analysis including both effects is a suitable topic for further research.

The general equations describing heat transport in a porous medium are rather complex. For the slow flows of interest here, it is reasonable to assume that the solid rock at a given position (with density $\rho_s$ and specific heat $C_{ps}$) has the same temperature as the fluid occupying its pores. Also, variation of front velocity $V$ with time is presumed to be slow enough to justify use of a quasi-steady state approach. With this assumption use of a coordinate system moving with velocity is convenient because the temperature distribution in the water region is then independent of time. When the appropriate equation for heat transport given by Bear (1972) is expressed in terms of the moving coordinate system with $z$ taken as the distance from the moving front, the result is

$$\left[\rho_2 C_{p2}\epsilon\left(\frac{V_2}{\epsilon} - V\right) - \rho_s C_{ps}(1-\epsilon)V\right]\frac{\partial T}{\partial z} = K_e \frac{\partial^2 T}{\partial z^2} \qquad (3)$$

$K_e$ in (3) is an effective thermal conductivity of the porous medium. Also $((V_2/\epsilon) - V)$ and $(-V)$ are the apparent velocities of water and rock respectively in the moving coordinate system.

The solution of (3) having $T = T_1$ at the front $z = 0$ and $T \to T_{2\infty}$ as $z \to \infty$ is

$$T = T_{2\infty} + (T_1 - T_{2\infty})e^{-\gamma z}$$
$$\gamma = \frac{\rho_2 C_{p2}\epsilon}{K_e}\left(V - \frac{V_2}{\epsilon}\right) + \frac{\rho_s C_{ps}(1-\epsilon)V}{K_e} \qquad (4)$$

The temperature profile is sketched in Figure 1.

An energy balance for the stationary region between lines A and B in Figure 1 yields the following equation:

$$\rho_1 V_1 H_1 - \rho_2 V_2 H_{20} + K_e \left.\frac{\partial T}{\partial z}\right|_0 = \epsilon V(\rho_1 U_1 - \rho_2 U_{20}) \qquad (5)$$

Here $H_i$ and $U_i$ are enthalpy and internal energy per unit mass for phase $i$. A subscript 0 indicates that the quantity is to be evaluated at the front. The heat flux term in (5) can, of course, be determined using (4).

Equations (2) and (5) can be solved simultaneously to obtain water velocity $V_2$ and front velocity $V$ in terms of the known steam velocity $V_1$. With the approximation $U_i = H_i$, which simplifies the final expressions while introducing an error of only a few percent in most cases, the results are

$$V = V_1 \frac{\rho_1(H_1 - H_{2\infty})}{\epsilon\rho_1(H_1 - H_{2\infty}) + (1-\epsilon)\rho_s C_{ps}(T_1 - T_{2\infty})} \qquad (6)$$

$$V_2 = V_1 \frac{\epsilon\rho_1(H_1 - H_{2\infty}) + \frac{\rho_1}{\rho_2}(1-\epsilon)\rho_s C_{ps}(T_1 - T_{2\infty})}{\epsilon\rho_1(H_1 - H_{2\infty}) + (1-\epsilon)\rho_s C_{ps}(T_1 - T_{2\infty})} \qquad (7)$$

Advance of the front requires heating of additional solid. Equation (6) shows, as would be expected, that the front moves more slowly under conditions when more steam must condense to heat a given volume of solid. Indeed, $V \to 0$ as the specific heat $C_{ps}$ of the solid becomes very large. In the other extreme of a rock with very small $C_{ps}$ or, more realistically, a situation with a small temperature difference $(T_1 - T_{2\infty})$, $V_2 \cong V_1$ and the front moves at the same velocity $(V_1/\epsilon)$ as that of the fluids advancing through the pore space. In this case, steam simply displaces water in the reservoir and no appreciable condensation occurs. Finally, it is noteworthy that $V$ is independent of the thermal conductivity $K_e$—at least for the present case where lateral heat losses to adjacent rock layers have been neglected.

The above equations are a special case of quite general models which have been developed to describe moving condensation fronts during steam drive oil recovery processes (for example, Mandl and Volek, 1969; Shutler, 1969). A relatively simple model of the initial flat front situation is desirable here because it allows the important physical effects to be seen in the following stability analysis without making the mathematics too complicated.

## STABILITY ANALYSIS

The displacement front, initially the plane $z = 0$ in the moving coordinate system, is now presumed to undergo a small wavy perturbation to the position $\overline{z} = \delta(t) f(x, y)$, where the function describing the wave form satisfies

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = -\alpha^2 f \quad (8)$$

The wave number $\alpha$ is $(2\pi/\lambda)$, where $\lambda$ is the mean wavelength of the perturbation. In accordance with the usual normal mode method for analyzing asymptotic stability of a small perturbation (Chandrasekhar 1961), the forms of the perturbations $\Theta$ in temperature and $\phi$ in the velocity potential are taken as products of $f(x, y)$, and appropriate functions $\varphi$ and $\theta$ of the distance $z$ from the front. The functions are dictated by the governing differential equations.

By taking the divergence of Darcy's Law and invoking continuity, it is readily shown that the velocity potential satisfies Laplace's equation, that is, $\nabla^2 \phi = 0$. The solutions which vanish far from the front are

$$\begin{aligned} \phi_1 &= a_1 e^{\alpha z} f(x, y) \\ \phi_2 &= a_2 e^{-\alpha z} f(x, y) \end{aligned} \quad (9)$$

The velocity perturbations can be obtained from (9) using $\underline{v}_i = \nabla \phi_i$.

The temperature perturbation $\theta(z)$ in the water phase can be obtained by solving the energy equation in the moving coordinate system. For the marginal stability condition which separates regions of stable and unstable behavior, the perturbation neither grows nor decays ($d\delta/dt = 0$), and the equation becomes

$$\left[\rho_2 C_{p2}\left(\frac{V_2}{\epsilon} - V\right) - \rho_s C_{ps}(1-\epsilon) V\right] \frac{\partial \theta}{\partial z} + \rho_2 C_{p2} v_{2z} \frac{\partial T}{\partial z} = K_e \left(\frac{\partial^2}{\partial z^2} - \alpha^2\right) \theta \quad (10)$$

When the initial temperature distribution $T(z)$ from (4) and the velocity perturbation $v_{2z}$ are substituted into (10) and the resulting differential equation is solved, the solution which vanishes far from the front is found to be

$$\begin{aligned} \theta &= a_3 e^{-\gamma_2 z} + \frac{(T_1 - T_{2\infty}) \rho_2 C_{p2} a_2}{K_e} e^{-(\alpha+\gamma) z} \\ \gamma_2 &= \frac{\gamma}{2} + \sqrt{\alpha^2 + \frac{\gamma^2}{4}} \end{aligned} \quad (11)$$

Along the wavy displacement front temperature is, to first order in perturbation amplitude, given by $[T(0) + \delta f T'(0) + f\theta(0)]$. The requirement that this expression must everywhere be equal to the saturation temperature $T_1$ leads to

$$-\gamma(T_1 - T_{2\infty})\delta + (\rho_2 C_{p2}/K_e)(T_1 - T_{2\infty}) a_2 = 0 \quad (12)$$

Mass and energy must also be conserved locally along the wavy front. Application of the former requirement at marginal stability gives

$$\rho_1 v_{1z} = \rho_2 v_{2z} \quad (13)$$

Similarly, conversation of energy implies

$$\rho_1 v_{1z} H_1 + K_e[T''(0)\delta + \theta'(0)] = \rho_2 v_{2z} H_{20} \quad (14)$$

The final boundary condition along the wavy front is a uniform pressure difference between phases. In each phase the pressure along the front is $[P_i(0) + \delta f P_i'(0) + f p_i(0)]$, where $P_i$ and $p_i$ are the initial pressure distribution and its perturbation. According to Darcy's Law, $(f p_i)$ is given by $(-\mu_i \phi_i / k_i)$. When the expressions given by (1) and (9) are employed, the boundary condition becomes

$$\frac{-\mu_2}{k_2}(V_2\delta + a_2) + \rho_2 g_z \delta = \frac{-\mu_1}{k_1}(V_1 \delta + a_1) + \rho_1 g_z \delta \quad (15)$$

With the velocity perturbations $v_{iz}$ written in terms of $a_1$ and $a_2$ using (9), Equations (12) through (15) are four linear, homogeneous equations in $a_1$, $a_2$, $a_3$ and $\delta$. For a nontrivial solution to exist, the determinant of coefficients for these equations must vanish, a requirement which leads to the following condition for marginal stability:

$$0 = -(\rho_2 - \rho_1) g_z \alpha + \alpha\left(-\frac{\mu_1 V_1}{k_1} + \frac{\mu_2 V_2}{k_2}\right) - \left(\frac{\mu_1}{\rho_1 k_1} + \frac{\mu_2}{\rho_2 k_2}\right) \frac{K_e \gamma (\gamma_2 - \gamma)(T_1 - T_{2\infty})}{(H_1 - H_{2\infty}) - C_{p2}(T_1 - T_{2\infty})\left(\frac{\gamma_2 - \gamma}{\alpha}\right)} \quad (16)$$

## INTERPRETATION OF STABILITY CONDITION

The three terms in (16) represent three effects on stability of the front. When any of the terms has a positive value, its effect is destabilizing and must be balanced at marginal stability by negative values (stabilizing effects) of one or more of the other terms. The first term represents the well-known effect of gravity, which acts to stabilize the front when the denser fluid lies below the lighter fluid. The second term represents fluid mechanical effects. For a simple displacement with no phase change $V_1 = V_2$ and this term simplifies to Saffman and Taylor's (1958) finding that a destabilizing effect exists when mobility $(k/\mu)$ of the displacing fluid 1 exceeds that of the displaced fluid 2. But in the present case, where a phase change does occur at the moving front, $V_1$ and $V_2$ are not equal but are instead related by (7). As steam density $\rho_1$ is less than water density $\rho_2$, it is clear from (7) that $V_2 < V_1$ and the front is more stable than would be predicted from mobility considerations alone. Effects of this type have not been included in previous analyses of stability in porous media.

That fluid experiencing a decrease in specific volume while crossing a moving front tends to stabilize the front is consistent with the analysis of Landau (1944). Actually, Landau was interested in moving flame fronts (with no porous medium involved) where fluid expands and thus acts to destabilize the front. Evidently, expansion promotes instability by adding mechanical energy while contraction favors stability by removing mechanical energy from the floor. For the present situation, the decrease in volume on condensation reduces water velocity $V_2$ relative to steam velocity $V_1$ as indicated above. The relationship between pressure gradients in the two phases is similarly affected. Hence, if a small element of steam enters the region originally occupied by water, it experiences a smaller pressure gradient acting to drive it farther into the water than it would if there were no volume change and $V_1$ and $V_2$ were equal.

The third term in (16) is a stabilizing effect due to heat transport in the water phase. It too is novel for stability analyses involving porous media. As mentioned previously, advance of the front requires heating the rock just ahead of it in the reservoir. At a point such as $P$ in Figure 2 along the wavy front, some of the heat released by condensation is transported laterally toward $Q$ and $R$. This lateral heat transport acts to decrease the rate at which rock is heated in advance of $P$ and to increase the rate at which rock is heated in advance of $Q$ and $R$, a stabilizing effect.

It is noteworthy that a similar effect acts to destabilize a moving interface during solidification of a pure material (see Sekerka, 1968). In this case interfacial speed is limited by the rate at which the heat of solidification can be transferred away from the interface into the liquid (region 2). Because of lateral heat transport away from a point such as $P$ in Figure 2, solidification can proceed faster there, a destabilizing effect.

For long wavelengths $((\alpha/\gamma) << 1)$, $(\gamma_2 - \gamma)$ approaches $(\alpha^2/\gamma)$ and, according to (16), the transport effect becomes very small relative to the gravity and fluid mechanical effects. This is the expected result because very little lateral transport occurs in this case. In contrast, for short wavelengths $((\alpha/\gamma) >> 1)$, $(\gamma_2 - \gamma) \cong \alpha$, all

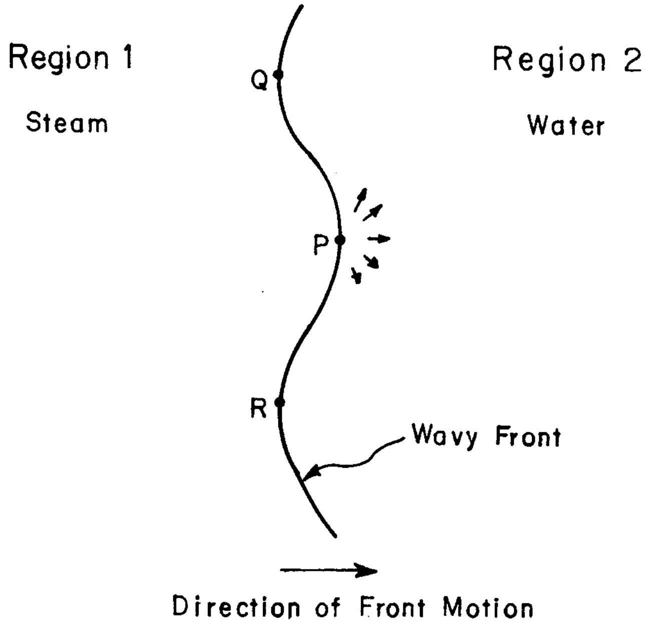


**Fig. 2. The effect of heat transport on front stability. At point *P* the rate of heat transfer to the water phase increases because of lateral heat transfer toward Q and R.**

three terms in (16) are proportional to $\alpha$, and the stabilizing effect of lateral transport can be significant.. Thus, it is possible to have situations where perturbations with long wavelengths are unstable, but perturbations with short wavelengths are stabilized by lateral transport. In this case there is presumably an intermediate wavelength which eventually dominates the instability because its growth rate is most rapid. The present analysis is limited to marginal stability, however, and so can provide no information about this fastest growing perturbation.

## NUMERICAL EXAMPLE FOR STEAM INJECTION PROCESS

A numerical example will illustrate that both the decrease in specific volume on condensation and the transport effect can significantly influence front stability. Suppose that water at a reservoir temperature $T_{2\infty}$ of 30°C is displaced by saturated steam at a temperature $T_1$ of 200°C. Under these conditions, steam viscosity is $1.6 \times 10^{-5}$ N·s/m$^2$, while water viscosity at reservoir temperature is $8.1 \times 10^{-4}$ N·s/m$^2$. Other properties of steam and water may be found in the steam tables. A vertical front is assumed so that gravity does not affect front stability. Finally, values of 0.2 for porosity $\epsilon$ and 794 J/kg·K for solid specific heat $C_{ps}$ are taken based on properties of sandstone.

Were one to assess front stability in this case considering the well-known effect of fluid viscosities described in Saffman and Taylor's (1958) paper but ignoring the volume change and transport effects considered here, he would conclude that the front should be highly unstable. The reason is that water viscosity is about 50 times greater than steam viscosity. If the volume change accompanying condensation is included, however, and if permeability $k$ is taken as the same in each phase, the second term of (16) becomes $(0.15\ \alpha\mu_1 V_1/k_1)$. Although, as indicated by the positive sign, the net effect of this term is destabilizing, the magnitude of the numerical coefficient is small. Thus, the stabilizing effect of the volume decrease accompanying condensation is large and is almost able to offset an adverse viscosity ratio of 50. Indeed, Equation (7) shows that $(V_2/V_1) = 0.023$ for the present example so that the volume decrease could stabilize a front with an adverse viscosity ratio of about 42 or less.

As indicated previously, the transport effect on front stability is negligible for disturbances with long wavelengths $(\alpha << \gamma)$. Stability is entirely determined by viscosity and volume change effects so that, as indicated above, the front is slightly unstable with respect to such disturbances for the present example. But for short wavelengths $(\alpha >> \gamma)$, the transport effect given by the third term of (16) becomes $(-1.4\ \alpha\mu_1 V_1/k_1)$. As the negative coefficient of this term exceeds in magnitude the positive coefficient 0.15 of the term discussed above, the front is stable with respect to perturbations having short wavelengths.

For some intermediate wavelength the value of $\alpha$ is such that the last two terms of (16) sum to zero and the front is marginally stable. This wavelength will have the same order of magnitude as $(1/\gamma)$, the distance in which water temperature ahead of the front falls from steam saturation temperature to (approximately) reservoir temperature. From (4) $(1/\gamma)$ is found to be in the range of a few meters for the present example if $K_e$ is taken as 5 J/m·s·K based on information given by Bear (1972, p. 650) and if typical oil field velocities of about $10^{-5}$ m/s are used. Thus, transport stabilizes all disturbances with wavelengths shorter than a few meters. Information of this type may be useful in designing and interpreting laboratory experiments on front stability. For example, if the size of the laboratory equipment is such that unstable disturbances of long wavelengths are precluded, observation of a stable front in the laboratory could give a misleading impression about front stability in the field where the unstable disturbances of long wavelengths can occur.

## DISCUSSION

The simple condensation and displacement process analyzed above is, of course, much less complex than what takes place during an actual oil recovery process using steam drive. The neglect here of gravity override effects, that is, preferential steam flow in the upper part of the medium, has been mentioned previously. Moreover, both oil and water are displaced in actuality so that two-phase flow exists in region 2 of Figure 1. The main effect of two-phase flow is to decrease the effective mobility (increase the effective viscosity) of region 2. Another factor not considered here is heat losses to nonporous strata above and below the oil-bearing layer. Such losses affect the temperature profile in the reservoir and also cause some condensation in the steam phase before it reaches the displacement front. If enough condensation occurs, two-phase flow of steam and water can exist in region 1 of Figure 1. Finally, variation of fluid viscosity in the region ahead of the condensation front where the temperature falls from saturation temperature $T_1$ to reservoir temperature $T_{2\infty}$ has been ignored.

In spite of these limitations, the analysis presented above is significant in that it clearly demonstrates the importance of including both volume change and transport effects—in addition to the well-known viscosity effect—in analyzing front stability during thermal recovery processes. The importance of these effects is also shown by existing experimental data. Baker (1973) describes laboratory experiments where stable condensation fronts were often observed during steam drive processes in spite of unfavorable viscosity (or, more precisely, mobility) ratios. For extremely viscous oils, however, the mobility ratio was so unfavorable that instability occurred in spite of the stabilizing effects of transport and volume decrease during condensation. In fact, Baker suggested that these effects might be responsible for his results although his discussion was entirely qualitative.

A recent paper (Connally and Marberry, 1974) describing a field test of a steam drive process is an indication of the practical importance of front stability. The authors conclude that front instability was the major limitation to process effectiveness during the test. It should be noted that, in addition to the effects considered here, reservoir inhomogeneities may have contributed to the development of front instability during the test.

While the above remarks have dealt with steam drive oil recovery processes, it should be emphasized that the present analysis provides new insight into the basic process of instability in porous media. The main conclusions are thus pertinent to a wide variety of situations. Displacement fronts between steam and water may be a feature of formations of interest in connection with utilizing geothermal energy. Both volume change and transport effects should have important influences on stability of moving reaction fronts during oil recovery processes involving underground combustion. Most of the experience with such processes involves situations where only air is injected into the reservoir. In recent years attention has shifted toward processes where air and water are injected simultaneously. In these wet combustion processes, injected water vaporizes at the moving reaction front. The destabilizing effect of this expansion could well be important so that inferences about front stability during wet combustion processes based simply on experience with ordinary dry combustion could be misleading.

Moving reaction fronts also occur in some cases of rapid chemical reaction in packed beds. Removal of an undesirable component such as $SO_2$ from a gas stream by fast reaction with bed particles is one example. Here too the effects described above could influence front stability.

## ACKNOWLEDGMENT

This work was supported by National Science Foundation Grant GK-38556.

## NOTATION

$C_p$ = specific heat, J/kg · K
$f$ = function describing spatial periodicity of perturbation
$H$ = enthalpy, J/kg
$k$ = permeability, $m^2$
$K_e$ = effective thermal conductivity of porous medium, W/m · K
$P$ = pressure before perturbation, $N/m^2$
$p$ = perturbation in pressure, $N/m^2$
$T$ = temperature, K
$U$ = internal energy, J/kg
$V$ = velocity of displacement front, m/s
$V_i$ = initial velocity in region $i$, m/s
$v_i$ = perturbation in velocity in region $i$, m/s
$x, y$ = coordinates in plane of unperturbed front, m
$Z$ = coordinate normal to front in stationary coordinate system, m
$z$ = coordinate normal to front in moving coordinate system, m

### Greek Letters

$\alpha$ = wave number, $m^{-1}$
$\gamma$ = term defined by Equation (4), $m^{-1}$
$\delta$ = amplitude of front displacement, m
$\epsilon$ = porosity, dimensionless
$\theta$ = perturbation in temperature, K
$\mu$ = viscosity, N · s/$m^2$
$\rho$ = density, kg/$m^3$
$\Phi$ = velocity potential before perturbation, m
$\phi$ = perturbation in velocity potential, m

### Subscripts

1 = region 1
2 = region 2
$s$ = solid (matrix of porous medium)
0 = evaluated at front
$\infty$ = evaluated in region 2 far from front
$z$ = $z$-component

## LITERATURE CITED

Baker, P. E., "Effect of Pressure and Rate on Steam Zone Development in Steamflooding," *Soc. Pet. Eng. J.*, **13**, 274 (1973).

Bear, J., *Dynamics of Fluids in Porous Media,* Elsevier, New York (1972).

Chandrasekhar, S., *Hydrodynamic and Hydromagnetic Stability,* Clarendon Press, Oxford (1961).

Connally, C. A., and J. E. Marberry, "Steam Flood Pilot, Nacatoch Sand—Troy Field, Arkansas," paper presented at Soc. Pet. Eng. Symp. on Improved Oil Recovery, Tulsa (1974).

Landau, L., "On the Theory of Slow Combustion," *Acta. Physiochem. URSS*, **19**, 77 (1944).

Mandl, G. and C. W. Volek, "Heat and Mass Transport in Steam-Drive Processes," *Soc. Pet. Eng. J.*, **9**, 59 (1969).

Miller, C. A., "Stability of Moving Surfaces in Fluid Systems with Heat and Mass Transport. II. Combined Effects of Transport and Density Difference Between Phases," *AIChE J.*, 19, 909 (1973).
———., and K. Jain, "Stability of Moving Surfaces in Fluid Systems With Heat and Mass Transport. I. Stability in the Absence of Surface Tension Effects," *Chem. Eng. Sci.*, 28, 157 (1973).
Saffman, P. G., and G. I. Taylor, "The Penetration of a Fluid into a Porous Medium or Hele-Shaw Cell Containing a More Viscous Liquid," *Proc. Roy. Soc.*, (London), **A245**, 312 (1958).
Sekerka, R. F., "Morphological Stability," *J. Cryst. Growth*, 3-4, 71 (1968).
Shutler, N. D., "Numerical Three-Phase Simulation of the Linear Steam Flood Process," *Soc. Pet. Eng. J.*, 9, 232 (1969).

*Manuscript received August 14, 1974; revision received and accepted December 11, 1974.*

# A New Method for Nonlinearly Constrained Optimization

**A new penalty function method of solving problems involving a nonlinear objective function subject to nonlinear equality and inequality constraints is described. It ameliorates difficulties experienced with the ill-conditioning of the Hessian matrix of classical penalty function methods. Experience based on the solution of 25 test problems indicates the proposed method is as good as, or better, than methods that are now being used.**

**J. S. NEWELL**
**and**
**D. M. HIMMELBLAU**
**Department of Chemical Engineering**
**University of Texas**
**Austin, Texas 78712**

## SCOPE

Chemical engineers frequently encounter realistic optimization problems that involve maximization or minimization of a cost, revenue, or other function subject to certain constraints. The constraints may be either equations, such as material or energy balances, or inequalities, such as capacity limits, or both. Often the objective function and constraints are nonlinear. A surprising number of practical chemical engineering problems have the characteristics just listed, such as the determination of steady state plant operating conditions, scheduling problems, capacity expansion analysis, some types of model building, and constrained regression. Furthermore, one of the most important steps in chemical engineering process design is the specification of the best values of the design variables according to some criterion.

Although the available techniques of optimization via numerical methods have multiplied exponentially in the last ten years with the advent of large-scale computers, most of the techniques prove to be ineffective when applied to solvable practical problems of the type outlined above. We describe here a method of minimizing a nonlinear objective function subject to nonlinear constraints that is efficient, robust, user oriented, and based on sound theoretical principles. The proposed technique is termed the General Augmented Penalty Function (GAPF) method in as much as it is one of a class of nonlinear optimization methods that employ penalties to accommodate the constraints in the problem.

## CONCLUSIONS AND SIGNIFICANCE

Although numerous algorithms have been proposed to solve constrained nonlinear optimization problems, surprisingly little is known about their relative merits. It is difficult for an engineer to isolate methods that are best suited for his problems. It has been demonstrated both theoretically and by numerical tests that the GAPF method in most instances alleviates the traditional numerical problems of penalty function methods while retaining their attractive features, such as the use of unconstrained minimization and the absence of a requirement to maintain feasibility as the optimization proceeds.

To demonstrate the performance of the proposed method relative to other algorithms that have been reported in the literature to be effective, the GAPF method was implemented in a computer code and tested on 25 problems of which 15 involved nonlinear constraints. One-half of the problems have their origin in the field of chemical engineering. It was found that the GAPF Code was both robust and quick, and outperformed the traditional penalty function methods. For the problems involving nonlinear equality constraints, the method was distinctly superior to all other methods. Data to support these conclusions is compiled. Because the computer code is easy to execute from the user's viewpoint and because the method essentially requires no arbitrary parameters to be selected by the user, it can be recommended for use by those who have only minimal experience with optimization techniques and "need to get the job done."