LETTERS TO THE EDITOR

To the Editor:

In a recent note, Pommersheim *et al.* (1980) used the Weierstrass-Erdmann (W-E) corner conditions of the calculus of variations (Miele, 1962) to call into question the optimal temperature policies for batch reactors with decaying catalyst found by Pommersheim and Chandra (1975) and Szepe and Levenspiel (1968).

In particular they claimed that no temperature policy is optimal, for the problems considered, which consists of an increasing temperature until the prescribed limit is reached and then of the constant upper temperature for the remainder of the time available. Their argument hinged on the assertion that a discontinuity in temperature as a function of time would contravene the W-E corner conditions.

Their argument is not valid for a *continuous* temperature policy with a discontinuity in its derivative with time (piecewise smooth policy) since all of the other variables involved in the W-E corner conditions are, or are equal to, solutions of differential equations—and hence continuous functions of time. All of the functions of such variables are continuous functions of their arguments and hence continuous functions of time. (See Bartle (1964)). Thus the W-E corner conditions are satisfied and piecewise smooth temperature policies cannot be excluded *a priori* as being non-optimal. Therefore, no evidence has been brought out to invalidate the optimal policies of Pommersheim and Chandra (1975) nor of Szepe and Levenspiel (1968).

Even their argument to exclude discontinuity in the temperature is not convincing since they do not discuss the sign and magnitude of λ_3 in arguing that C in their Eq. 32 cannot have the same value for two different temperatures.

If it can be shown that C is a strictly monotonic function of temperature then a discontinuity in the optimal temperature policy at a particular time can be ruled out. Otherwise a quite careful argument is required to be able to exclude the discontinuity.

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To the Editor:

Dr. Crowe has pointed out in his letter that "all of the variables involved in the W-E corner conditions are, or equal to, solutions of differential equations—and hence continuous functions of time. . . ." Thus the W-E corner conditions are satisfied and piecewise smooth temperature policies cannot be excluded *a priori* as being nonoptimal." Accordingly he concludes that "no evidence has been brought out to invalidate the optimal policies of Pommersheim and Chandra (1975) nor of Szepe and Levenspiel (1968)." However, for the end conditions of maximizing conversion, given a final run time and a final activity, as studied by Szepe and Levenspiel (1968) and by Pommersheim and Chandra (1975), the optimal temperature policy is a monotonically increasing one, i.e., neither a falling nor an isothermal temperature policy subarc can be a solution of the Euler-Lagrange equations for any given set of initial values. Hence, λ_{i+} and C_+ (pertaining to the isothermal subarc) in the W-E corner condition (Eqs. 28 and 29 of Pommersheim *et al.* (1980)) are not solutions of the Euler Lagrange equations. The argument that these are continuous solutions of differential equations at the corner is hence erroneous and the W-E corner conditions are not satisfied.

Further he states that our argument to exclude a discontinuity in temperature is not convincing. A "jump" discontinuity in the optimal temperature policy would result in a jump in the λ_i values at the corner. This violates the W-E corner condition, Eq. 28. Further such a subarc with dy/dt unbounded can be a solution of the Euler-Lagrange equations only as either concentration and/or activity is driven to zero.

With reference to the last paragraph of Dr. Crowe's letter, it must be remembered that over each subarc of the optimal policy, C, the integration constant, is precisely a constant, and hence not a function of temperature. This point has no basis. In actuality we can only solve for λ_i/C in terms of kinetic parameters. Therefore, one only needs to check the corner condition in terms of λ_i/C.

It should be noted that any policy is not an overall optimal policy unless it satisfies the transversality condition as demanded by the requirement that variation should vanish on the boundary (Schechter, R. S., (1967)). Hence a trial and error on the initial temperature is needed both to keep the final temperature less than or equal to the prescribed maximum temperature and to satisfy the transversality condition. Similar conclusions, with respect to the optimization of packed bed reactors, are arrived at by Levenspiel and Sadana (1978).

Finally we would like to emphasize that our conclusions regarding the differences in optimal policies for different optimization criteria and the equivalence of the policies for some multiple reactions remain untouched by this discussion.

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To the Editor:

Recently, Chiou and Gordon published a paper entitled "Low Shear Viscosity of Dilute Polymer Solutions", *AIChE J.*, **26**, 852 (1980). They have reported the viscosity—pH curves of three different aqueous polymer solutions, which demonstrated that the addition of acid (i.e., hydrochloric acid) or base (i.e., sodium hydroxide) to deionized water results in a decrease of the low shear rate viscosity value of aqueous polymer solutions.

Recent results produced in our laboratory using *tap water* (see Table 1 of chemical analysis) show very similar trends to those reported by Chiou and Gordon. Controlled amounts of H_3PO_4, NaOH and NH_4OH, ranging from 20 to 1,000 wppm were added to tap water and subsequently aqueous solutions of polyacrylamide (Separan AP-273, Dow Chemical) in 1,000 wppm were prepared. The resulting viscosities measured over a wide range of shear rates (10^{-2} to 10^3) are presented in Figures 1 as a function of the measured pH value.

These viscosity—pH curves show a maximum in the viscosity at a pH of approximately 10 for all values of the shear rate. However, at high shear rates of the order of 1,000 sec^{-1} corresponding to the range of capillary tube measurements, there is much less variation of the viscosity with pH as Chiou and Gordon point out. Figure 2 clearly shows that the low shear rate viscosity of deionized water solution is greater than that of tap water solution by a factor of 20, while at high shear rates the difference is much smaller.

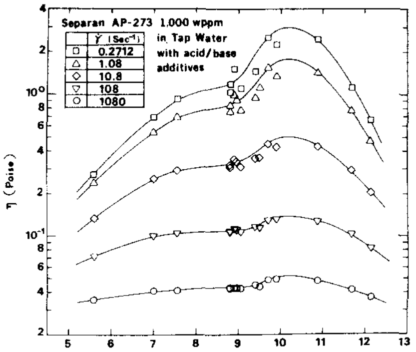

Figure 1

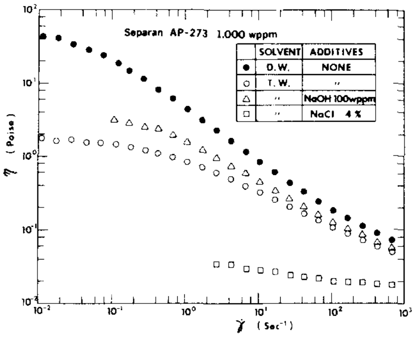

Figure 2

These results emphasize that the low shear rate rheology is very sensitive to the water chemistry. It should be noted as well, that for a given water chemistry the rheology of an aqueous polymer solution is dependent on the chemistry of the polymer which varies from batch to batch.

These considerations are of special significance in the study of the fluid mechanics and heat transfer performance of aqueous solutions of polymer inasmuch as an increase of the low shear rate viscosity is generally associated with a reduction in the friction factor and heat transfer in turbulent channel flows.

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TABLE 1. COMPREHENSIVE CHEMICAL ANALYSIS OF WATER

	$CaCO_3$	SO_4^{--}	Cl^-	Ca^{++}	Mg^{++}	K^+	Na^+	O_2
wppm	106	25	11	37	9	1.0	5.3	8.7

The pH value at 20°C is 8.0.