The Dynamics of Heat Removal from a Continuous Agitated-Tank Reactor

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The present investigation is concerned with the dynamic characteristics of a 12-in. diameter continuous agitated-tank reactor vessel. Response of the vessel effluent temperature to a change in coolant flow rate through an internal cooling surface is the subject of theoretical and experimental study. Experimental data were obtained through the use of frequency and transient response techniques. Studies were made for the passage of vessel-charge fluids with widely differing physical properties. Also data were taken for various conditions of fluid turbulence both inside and outside the internal heat transfer coils. Experimental and theoretical results are graphically compared. Recommendations are presented for the development of theoretical dynamic relationships.

Systems-engineering techniques are becoming increasingly important in chemical-process development and control. The first step required is a theoretical analysis of the process in question from the standpoint of unsteady state behavior. For all but the simplest of processes such analyses generally yield differential equations describing the dynamic behavior of the given process. One method of profiting from these equations is by electronic simulation. The equations, along with those describing *controller action*, are programmed into an analogue computer, to simulate the process with its attendant controls. Changes in the response of desired output variables may be observed for different controller settings, flow rates, feed concentrations, equipment sizes, etc. As such simulation techniques become more highly developed, the quantity of chemical-process pilot-plant data customarily necessary may be greatly reduced. For certain types of problems a complete elimination of pilot-plant data can be expected. In addition, information vital to advanced process-control methods is made available.

In the development of equations suitable for analogue-computer programming a number of simplifying assumptions and approximations are generally needed. The validity of certain equations employed may then be open to question. The object of the present investigation is to carry out a theoretical study of the dynamics of heat removal from a continuous agitated-tank reactor. The theoretical equations developed differ because of the various assumptions made in their derivation. Experimental data are then taken to confirm the equation most desirable for a particular set of process conditions. If enough information of this type is made available by further experimentation, process simulation will proceed at a faster rate, with more assurance of accuracy in the final results.

Many reactors of the batch or agitated-tank type are jacketed, with the inner tank walls serving as a heat-exchange surface. Newer designs have utilized the advantages of internal heat transfer surface together with proper agitation and baffling to provide favorable flow patterns and more effective heat transfer. The present equipment is designed along such lines with helical coils as the internal heat-exchange surface. Since most reactions carried out in continuous, agitated-tank type of units are exothermic, this paper is devoted only to the dynamics of equipment heat removal. The dynamics of the given system are characterized by the comparison of experimental frequency-response data with theoretically derived transfer functions.

REVIEW OF PREVIOUS WORK

The literature relative to the analysis of process-control equipment by the use of servo-theory techniques is not abundant, because the interest of chemical engineers in this field is recent. Virtually all work with frequency-response methods in process equipment has been reported since 1953. Perhaps the earliest account of frequency-response analysis of a chemical unit operation was presented by Stanton and Hoyt on the dynamics of a fractionating column (*8*). In the heat transfer field McKnight and Worley described the analysis of a plate heat exchanger by frequency-response methods (*6*). Cohen and Johnson, as well as Mozley, investigated the dynamics of concentric-pipe heat exchangers (*3*, *7*). Williams and Young investigated the closed-loop dynamics of a multipass commercial type of heat exchanger with attendant control system by means of electronic simulation (*9*).

No complete work is available relative to the particular type of equipment under investigation. Mason presents an early mathematical study of the transients involved in a continuous-flow, steam-heated kettle (*5*). The transfer-function concept was not then in common use, and all solutions were carried out by classical means. Aris and Amundson, as well as Bilous, Block, and Piret, presented recent studies of the dynamics of a continuous agitated-tank reactor (*1*, *2*). In these papers a number of theoretical transfer functions were derived and studied by plotting on a Nyquist diagram. Both articles were theoretical, and no experimental data were taken.

The present work differs from most of the previous efforts on continuous tank type of systems, as emphasis is placed upon experimental data. The investigation consists of a theoretical analysis with accompanying experimental confirmation of the dynamics of a continuous, agitated-tank reactor during removal of sensible leat. The experiments were made with oil and water used as charge fluids and water used as the cooling medium. In all cases the output variable was taken as the tank fluid temperature, while the input or forcing variable was cooling-water flow rate.

DESCRIPTION OF EQUIPMENT AND EXPERIMENTAL METHODS

Process Equipment

In the dynamic analysis of a type of equipment or process the object is to obtain a valid relationship between the desired input variable, the output variable which it affects, and time. Such a relationship is usually referred to as the *open-loop* or *process-transfer* function and is essential to a complete understanding of the feedback loop later installed to control the output variable in question. Usually the process-transfer function is defined in terms of the Laplacian complex variable instead of time. Compatibility with modern servo-control theory is thereby assured.

Figure 1 shows a schematic flow diagram of the apparatus used in the investigation. Hot feed is pumped to the agitated tank. Effluent passes by means of a siphoning effect into the discharge barrel for reuse during subsequent runs. Water coolant flows into the bottom of the tank, through helical coils, then to discharge. The coolant flow rate may be forced in a periodic manner by a sine-wave generator mounted on the discharge side of the coolant stream. Both feed and coolant streams are measured accurately by calibrated rotameters.

With the exception of the sine-wave

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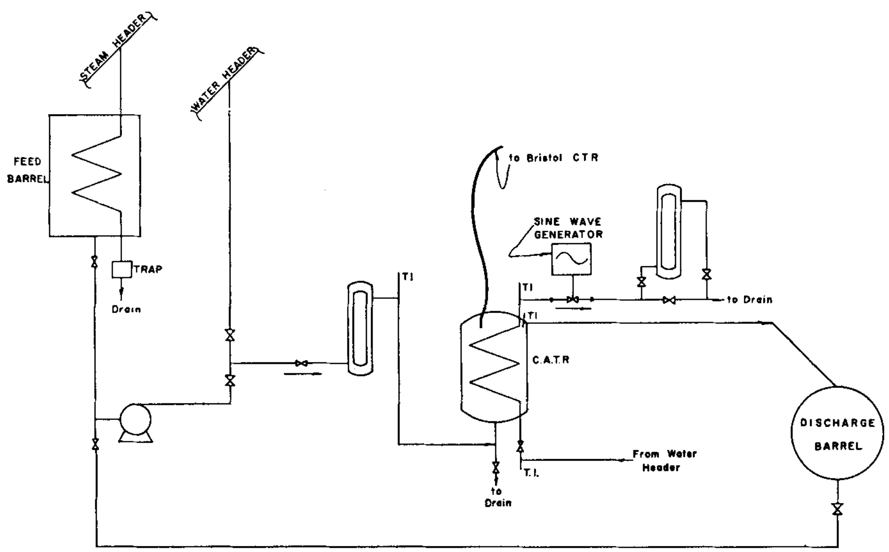

Fig. 1. Flow diagram of equipment.

generator all equipment is quite conventional. The tank reactor vessel is a stainless steel cylinder 12 in. in diameter and 15 in. high. It is provided with a turbine type of impeller with 4-in. diameter blades. Agitator speeds are continuously adjustable from 70 to 1,750 rev./min. Tank baffling consists of 1-in. stainless steel strips extending the height of the tank and spot welded 90 deg. apart. The tank is heavily insulated on top and bottom with plywood and on the sides with 2-in. fiber glass. The helical heat transfer coil, 5 in in diameter, is constructed from ⅝ in., type-L copper tubing. The output variable, which is the instantaneous temperature within the tank, was recorded continuously by means of a Bristol model-560 recording potentiometer with a strip chart.

Sine-Wave Generator

To obtain frequency-response data some method must be at hand to force the desired process variable in a sinusoidal manner. For a change in liquid flow rate such a periodic movement may be accomplished with reasonable accuracy by the use of a stop watch and flow-indicating device. However beyond a frequency of about 1.5 cycles/min., hand methods result in too much wave distortion. Some relatively simple, inexpensive device had to be developed which would permit oscillations up to 5 cycles/min. or higher if necessary. The most satisfactory arrangement consisted of a linear motor control valve with the stem driven by a small, geared-down induction motor.

The basic portion of the sine-wave generator consists of a ½-in. research control valve. The trim is stainless steel, and the valve body is bronze with a 150 lb./sq. in. gauge working pressure. Trim bevel is such that the valve is linear through the lower 80% of stem travel. Extensive test data taken at constant pressure drop show this to be true *(4)*. In the construction of the generator the top half of the diaphragm body was removed together with diaphragm and spring. The cast-aluminum housing, which had served as the lower half of the diaphragm body was then used to support the device which imparted a harmonic translational motion to the valve stem. This device is made up of a rotational power source and Scotch yoke together with connecting gears. The driver consists of a Merkle-Korff SG-10 induction motor attached to a gear reduction housing. Motor gear-train output speed is 1 rev./min. and maximum output torque is 10 lb.-in. Appropriate gear sets connect the motor-output drive to the Scotch-yoke drive. The arrangements of gears are such that yoke-drive speeds of 0.1, 0.25, 0.5, 1.0, 2.5, and 5 cycles/min. are obtainable. The range can easily be increased by exchange with a motor of higher speed. The free end of the valve stem is screwed into the Scotch-yoke drive block and secured by lock nut. Variable, periodic motion is thereby imparted to the valve stem. Since the valve trim is linear, as proved by test, throughout the bottom portion of its movement, a sine wave of fluid flow passes through the valve body. A variable amplitude of stem movement, and therefore fluid flow rate, is obtained by the installation of yoke-drive throws of varying radii. Throughout most of this work a peak-to-valley stem travel of ⅛ in. was used. The valve-plug location for steady state operation is continuously adjustable.

EXPERIMENTAL

The determination of steady state process gains were of key importance in this investigation. Such transient curves give a good indication of system order and amount of deviation from linearity and provide a basis for standardizing magnitude ratios. A step increase in coolant flow rate yielded a negative gain transient; a step decrease yielded the positive transient. The magnitude ratio may be mathematically defined as

Magnitude ratio

$$= \frac{\left(\frac{\Delta\theta}{\Delta W_w}\right)_{F=F}}{\left(\frac{\Delta\theta}{\Delta W_w}\right)_{F=0}} \tag{1}$$

This equation may be easily simplified when it is considered that ΔW_w for a given response spectrum was a fixed quantity at all frequencies. Thus the equation may be effectively reduced to

Magnitude ratio

$$= \frac{(\Delta\theta)_{F=F}}{(\Delta\theta)_{F=0}} \tag{1a}$$

The numerator of this expression represents the average total distance between

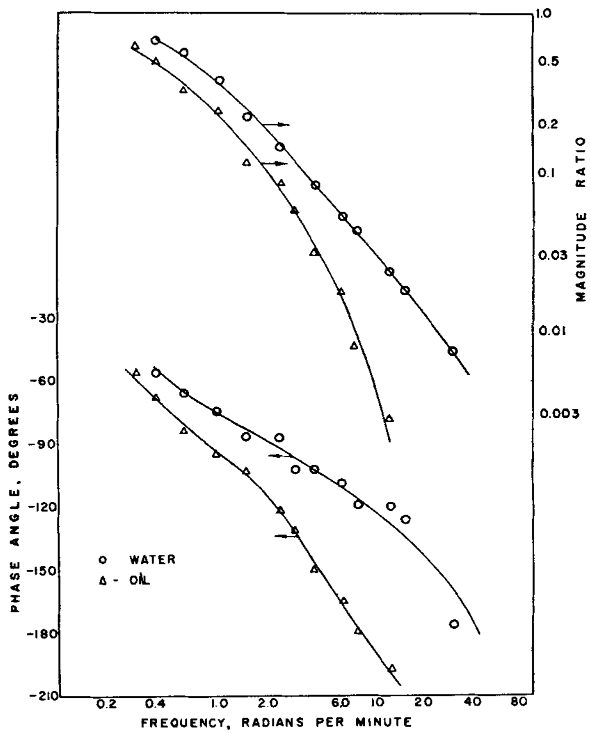

Fig. 2. Bode diagram comparing oil and water frequency-response curves.

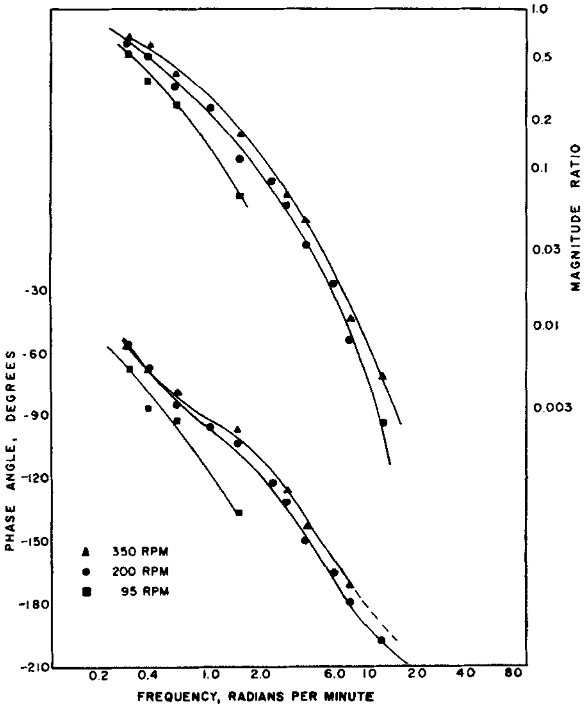

Fig. 3. Effect of tank-fluid conditions on frequency-response curves.

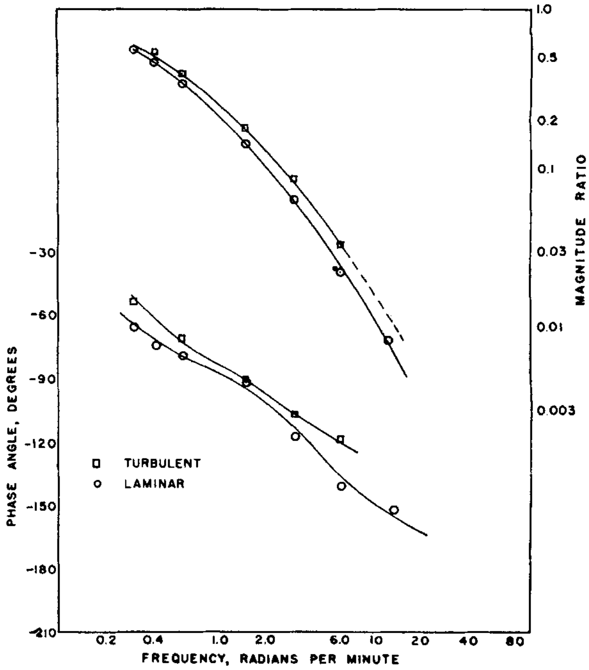

Fig. 4. Effect of coolant-flow conditions on frequency-response curves.

peaks and valleys of the output wave at any frequency F. The denominator represents the numerical sum of the positive and negative steady state process gains. Although this method of analyzing frequency-response data (magnitude ratio, phase angle, frequency) differs somewhat from procedures used previously, it has proved to be satisfactory. Phase angles were established by averaging the time in degrees between corresponding points on input and output waves.

VARIOUS EFFECTS ON SYSTEM DYNAMICS

The bulk of experimental work to date on the dynamics of process equipment has considered only one given set of process parameters. It may be intuitively deduced that the dynamics of heat removal for the given equipment would vary appreciably depending on the type of material processed. The amount of deviation between water and oil is shown by the attenuation and phase-lag curves in Figure 2. The oil used was a special low-viscosity-index material with a viscosity at room temperature comparable to S.A.E. 10 oil. It is seen that the dynamic-response characteristics of a given piece of equipment may be altered significantly according to the type of material being processed.

The effect, if measurable, of different conditions of tank-fluid turbulence upon system response was studied. Oil was selected as the process fluid because of its heavy outside controlling film. Agitator speeds of magnitudes that would yield Reynolds numbers for mixing equal numerical distances apart were selected for experimental parameters. Figure 3 shows the results of such frequency-response determinations. It is seen that the two higher agitator speeds yield curves which are quite close; however there is a decided drop in response for the lower speed. As a rule of thumb it may then be stated that, beyond Reynolds numbers of about 2,800 the effect on response of this equipment type is relatively small.

In addition to the effect of fluid conditions existing in the tank itself, it was also desirable to determine the change in equipment-response characteristics brought about by different fluid-flow conditions within the cooling coils. With the existing system it was not possible to maintain other parameters constant while varying flow conditions within the coils from laminar to turbulent types; however the deviations were relatively small. For the laminar flow response data, cooling-coil Reynolds numbers varied from 1,690 to 339, respectively, at the peaks and valleys of the input waves. Because of conduit configuration completely laminar flow probably did not exist over this entire range. The turbulent-flow response data were taken with coolant-flow Reynolds numbers which varied from 3,494 to 2,025. The average tank-fluid temperature was approximately 15° lower for the turbulent-flow response data. Because of its less dominant outside fluid film, water was selected as the process fluid. The results of this experimentation are summarized by the curves shown in Figure 4. As may be expected, equipment response is somewhat faster during conditions of turbulent flow within the cooling coils, all other variables remaining essentially constant. However the amount of change is not great.

DERIVATION OF THEORETICAL TRANSFER FUNCTIONS

As indicated by Figure 1, hot reactor feed is continuously pumped through the system, while a portion of its heat is removed by cooling water flowing through internal coils. It is desirable to study the dynamics of heat removal as a result of a change in coolant rate of flow (or bulk velocity). Throughout all runs the temperature signal was produced from a bare thermocouple junction, thus obviating any considerations regarding thermocouple-well lags. The true-temperature history of the cooling water must be represented by a partial-differential equation, as its temperature changes with time as well as length traversed. Using the method of finite differences applied to an unsteady state heat balance over a small coil section, one can obtain the following partial, nonlinear differential equation:

$$\frac{\partial \theta_w}{\partial t} + \frac{\partial \theta_w}{\partial X} V + \frac{1}{T_1} \theta_w = \frac{1}{T_1} \theta \qquad (2)$$

To obtain the transfer function desired, $\theta/W_w(j\omega)$, the partial derivative $\partial\theta_w/\partial X$ must be assigned a constant value, since in this case the forcing function is the coolant velocity. Another approach consists of the definition of a single cooling-water temperature in the following manner:

$$\bar{\theta}_w \triangleq \frac{\theta_{w_i} + \theta_{w_o}}{2}$$

or

$$\theta_{w_o} = 2\bar{\theta}_w - \theta_{w_i} \qquad (3)$$

The defining differential equation is then reduced to the linear, ordinary type. The key assumptions considered in developing the first of two theoretical derivations are as follows:

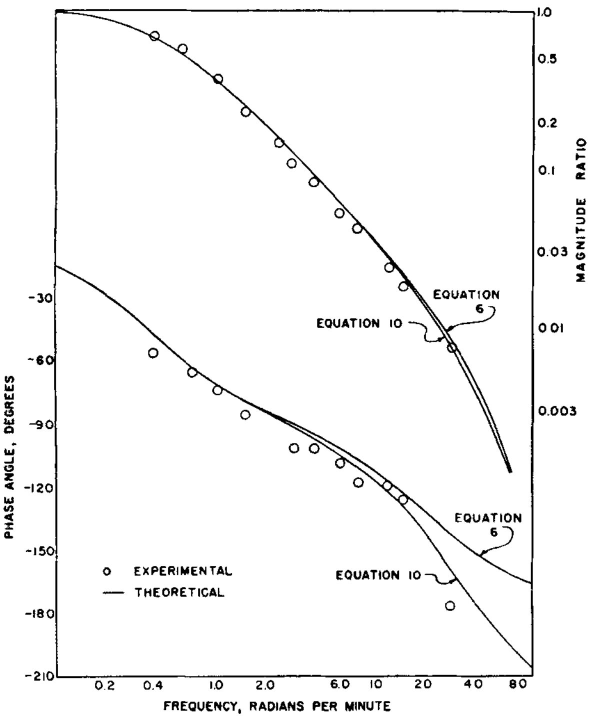

Fig. 5. Experiment and theoretical Bode diagrams, water.

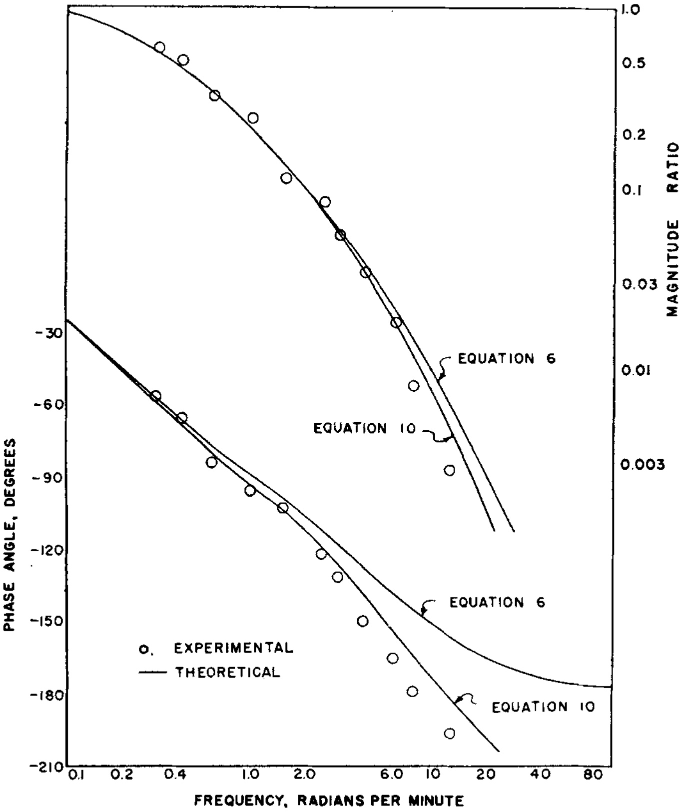

Fig. 6. Experimental and theoretical Bode diagrams, oil.

1. All metal capacitances are ignored as negligible in affecting the dynamics of heat removal. The two capacitances taken into account are those of the vessel fluid and the cooling-water holdup.

2. An over-all heat transfer coefficient is employed. Its value is assumed to be constant during the sinusoidal fluctuation of cooling-water flow rate and equal numerically to its value at mean steady state conditions.

Equations (4) and (5) are then transformed by the Laplace transformation with the condition that all variables are at zero variation from steady state conditions at $t = 0^+$. After the solution simultaneously and substitution of j^ω for the Laplacian complex variable the final form of the first theoretical transfer function is obtained as

$$\frac{\theta}{W_w}(j\omega) = \frac{2K_1/T_6}{(j\omega)^2 + (T_4 + T_7/T_4T_7)j\omega + 1/T_4T_7 - 1/T_3T_6} \tag{6}$$

Again by a dynamic heat balance over the cooling water with a coolant temperature as defined by Equation (3) used, the following relationship is obtained by finite difference techniques:

$$\frac{d\bar{\theta}_w}{dt} + \frac{\bar{\theta}_w}{T_4} - \frac{1}{T_3}\theta = 2K_1W_w \tag{4}$$

where

$$T_2 = \frac{C_w}{\bar{W}_wc_p}, \quad T_3 = \frac{C_w}{UA_a},$$

$$\frac{1}{T_4} = \frac{2}{T_2} + \frac{1}{T_3}, \quad K_1 = \frac{\theta_{wi}c_p}{C_w}$$

By similar methods of dynamic heat balance the following expression is derived for the tank fluid:

$$\frac{d\theta}{dt} + \frac{1}{T_7}\theta = \frac{1}{T_6}\bar{\theta}_w \tag{5}$$

where

$$T_5 = \frac{C_f}{W_fc_p}, \quad T_6 = \frac{C_f}{UA_a},$$

$$\frac{1}{T_7} = \frac{1}{T_5} + \frac{1}{T_6}$$

Completion of this mathematical operation has required the assumption of essentially linear-system characteristics for small excursions of the forcing and output variables about their mean steady state values. The treatment has produced a relatively simple second-order transfer function with a limiting phase lag of −180 deg. Comparison with experimental results will indicate whether or not the assumptions made in its derivation are justifiable.

The second derivation differs from the first in that individual film coefficients are considered along with another capacitance. The key assumptions are as follows:

1. The internal metal heat transfer coil offers sufficient lag so as to affect control dynamics at the medium and higher frequencies. All other metal capacitances are neglected.

2. The outer film coefficient of heat transfer remains constant during dynamical operation and equal numerically to its value at mean steady state conditions.

3. The inside film coefficient of heat transfer remains constant during sinusoidal fluctuations of flow rate and equal numerically to its value at steady state conditions.

When one applied the assumptions as outlined, together with a cooling-water temperature as defined by Equation (3), the following differential equations were derived when dynamic balances were made over the cooling water, heat transfer coils, and tank fluid:

Cooling water

$$\frac{d\bar{\theta}_w}{dt} + \frac{1}{T_{12}}\bar{\theta}_w - \frac{1}{T_8}\theta_c = 2K_1W_w \tag{7}$$

Coils

$$\frac{d\theta_c}{dt} + \frac{1}{T_{13}}\theta_c = \frac{1}{T_9}\theta + \frac{1}{T_{10}}\bar{\theta}_w \tag{8}$$

Tank fluid

$$\frac{d\theta}{dt} + \frac{1}{T_{11}}\theta = \frac{1}{T_{11}}\theta_c \tag{9}$$

New time constants are defined by

$$T_8 = \frac{C_w}{h_iA_i}, \quad T_9 = \frac{C_c}{h_oA_o},$$

$$T_{10} = \frac{C_c}{h_iA_i}, \quad T_{11} = \frac{C_f}{h_oA_o}$$

$$\frac{1}{T_{12}} = \frac{2}{T_2} + \frac{1}{T_8}, \quad \frac{1}{T_{13}} = \frac{1}{T_9} + \frac{1}{T_{10}}$$

Equations (7), (8), and (9) are transformed as before and solved simultaneously for the required transfer function. The final equation is

$$\frac{\theta}{W_w}(j\omega) = \frac{2K_2K_3/T_{11}}{A(j\omega)^3 + B(j\omega)^2 + C(j\omega) + D} \tag{10}$$

where

$$K_2 = \frac{T_{13}}{T_{11}}, \quad K_3 = \frac{T_{13}}{T_9},$$

$$\frac{1}{T_{14}} = \frac{1}{T_5} + \frac{1}{T_{11}}$$

$$A = T_{13}$$

$$B = \frac{T_{13}T_{12} + T_{14}(T_{13} + T_{12})}{T_{12}T_{14}}$$

$$C = \frac{T_{12} + T_{13} + T_{14}}{T_{12}T_{14}} - \left(\frac{K_2}{T_8} + \frac{K_3}{T_{11}}\right)$$

$$D = \frac{1}{T_{12}T_{14}} - \left(\frac{K_3}{T_{12}T_{11}} + \frac{K_2}{T_8T_{14}}\right)$$

COMPARISON OF THEORETICAL AND EXPERIMENTAL RESULTS

To prevent misinterpretation caused by meager and widespread data in the comparison of theory and experiment, about twice as many frequencies were tested as was normally the case. Detailed, original, numerical data are available for all runs (*4*). The sinusoidal value of the output temperature was examined very carefully, especially for phase-lag angles. As a rule a sharper contrast exists in theoretical phase-lag curves as compared with magnitude-ratio curves. All data were taken at an agitator speed of 200 rev./min. and with turbulent-flow conditions existing within the coils.

The theoretical curves are referred to by equation number in Figures 5 and 6. These response curves are for water and oil, respectively. Experimental points are denoted as before with small circles. With water as the process fluid both theoretical lag curves show pronounced leveling tendencies at -90 deg. before continuing on to their respective limiting phase angles of -180 and -270 deg. Such behavior indicates a dominant first-order response at the low and medium frequencies; however the experimental attenuation and phase-lag data show a definite multiorder response at the higher frequencies.

In contrast Equation (10) for oil as the process fluid is practically a straight line up to a lag of -120 deg. Here it curves downward and approaches its limiting-phase angle. Theoretical Equation (6), describing phase-lag loci for oil, reacts in somewhat the same manner except for a slight leveling tendency at -90 deg. and a limiting-phase angle of -180. From the theoretical and experimental investigation it may be concluded that the response of tank-fluid temperature to a change in coolant flow rate is definitely of higher order. Within limits of engineering accuracy a second-order transfer function [Equation (6)] represents the response for water over most of the frequency spectrum; however for oil the third-order expression [Equation (10)] is definitely recommended.

At the higher frequencies the original data were carefully examined for resonance as predicted by the theoretical descriptive equations for a concentric-pipe heat exchanger in the paper by Cohen and Johnson (*3*); no evidence of resonance was detectable, probably because the ouptut variable, tank-fluid temperature, represents the condition of a completely lumped medium. An authoritative discussion of the phenomenon of resonance may be found in reference *3*.

CONCLUSIONS

The dynamics of heat removal in a continuous agitated tank has been examined theoretically and comparison made with experimental response data. In all cases the forcing variable was coolant flow rate rather than coolant temperature, a fact which is of more interest from a practical control standpoint. The importance of fluid conditions, both inside and outside the heat transfer boundary, has been demonstrated graphically. The Reynolds number for mixing has been established at which response for the given system is significantly affected. Equations which are suitable for ease in adaptation to an analogue computer have been derived which compare favorably with experiment.

Experimental data have shown that little error is introduced by considering all coefficients of heat transfer as constants at mean steady state conditions. Numerical values for the various film coefficients have been calculated from existing correlations developed from data taken during steady state conditions. These are shown to be adequate for the case of transient operation.

Some of the more recent types of continuous agitated-tank reactor-control systems remove heats of reaction by the use of the latent heat of vaporization of a volatile coolant. Of considerable interest would be the development of transfer functions relating reactor-fluid temperature to coolant back pressure, since the latter is normally the variable manipulated in effecting temperature control. Together with information now available, the basis would thus be laid for a comprehensive study of continuous tank types of systems which would include a theoretical and experimental investigation devoted to open-loop dynamics for the case of an autothermic source within the reactor fluid.

NOTATION

A = surface area, sq. ft.
C = heat capacitance, $(M)(c_p)$, B.t.u./°F.
c_p = specific heat, B.t.u./(lb.)(°F.)
d = tube diameter, ft.
F = frequency, cycles/min.
h = individual heat transfer coefficient as obtained from established correlations for similar equipment, B.t.u./(min.)(sq. ft./°F.)
h_o = outer film coefficient of heat transfer
h_i = inside film coefficient of heat transfer
j = $\sqrt{-1}$
$L[f(t)]$ = $\int_0^\infty f(t)e^{-st}\,dt$
M = mass, lb.
s = Laplacian complex variable
T = time constant, min.
T_1 = $A_s\rho C_p/U\pi\, d$
t = time, min.
U = over-all heat transfer coefficient, B.t.u./(min.)(sq. ft./°F.)
V = coolant bulk velocity, ft./sec.
W = fluid flow rate, lb./min.
X = distance in direction of flow

Greek Letters

Δ = small change in process variable around the steady state
$\theta, \theta_c, \theta_w$ = vessel-effluent temperature, coil temperature, and coolant temperature, respectively
ω = imposed frequency, radians/min.
ρ = density, lb./cu. ft.

Subscripts

a = average area
c = coils
f = process fluid
i = inside area
o = outside area
s = sectional area
w = coolant
w_i = coolant in
w_o = coolant out

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