MODELING OF THE WSTF FRICTIONAL HEATING APPARATUS IN HIGH PRESSURE SYSTEMS

Final Report

NASA/ASEE Summer Faculty Fellowship Program 1992

Johnson Space Center

Prepared by: Christopher T. Skowlund, Ph.D.

Academic Rank: Assistant Professor

University & Department: New Mexico State University
Chemical Engineering Department
Las Cruces, New Mexico 88003

ABSTRACT

In order to develop a computer program able to model the frictional heating of metals in high pressure oxygen or nitrogen a number of additions have been made to the frictional heating model originally developed for tests in low pressure helium. These additions include: 1) a physical property package for the gases to account for departures from the ideal gas state, 2) two methods for spatial discretization (finite differences with quadratic interpolation or orthogonal collocation on finite elements) which substantially reduce the computer time required to solve the transient heat balance, 3) more efficient programs for the integration of the ordinary differential equations resulting from the discretization of the partial differential equations and 4) two methods for determining the best-fit parameters via minimization of the mean square error (either a direct search multivariable simplex method or a modified Levenburg-Marquardt algorithm). The resulting computer program has been shown to be accurate, efficient and robust for determining the heat flux or friction coefficient vs. time at the interface of the stationary and rotating samples.

INTRODUCTION

The frictional heating apparatus at WSTF is used to determine the flammability of various metals undergoing frictional heating in oxygen-rich environments. A detailed description of this apparatus has been given elsewhere[1] as well as a list of the previous mathematical models for the frictional heating.[2]

As a part of the 1991 NASA/ASEE Summer Faculty Fellowship Program a computer model[2] of the frictional heating apparatus was developed for frictional heating experiments in low pressure helium (approximately 75 psia). The model that was developed was successful in accurately fitting the experimental data for the helium via a best-fit of the friction coefficient or heat production at the interface of the rubbing samples.

The success of the model for the simplest case (i.e., a low pressure non-reactive gas) led to the hope that similar results could be achieved in much more difficult situations (i.e., a high-pressure reactive gas). The goal of this project was therefore to expand the low pressure model to include high pressure oxygen and nitrogen systems (at least up to 1,000 psia).

MODEL DEVELOPMENT

The model used in this study is the same transient one-dimensional equation for heat conduction as in the original model.[2] For each annular sample (i = 1,2) we have the following energy balance

$$\rho_i C_{p,i} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} k_i \frac{\partial T}{\partial x} - Q_v - Q_c - Q_r \qquad (1)$$

where ρ_i = the density of sample i, $C_{p,i}$ = the heat capacity of sample i, T = temperature in the sample, t = time, x = axial position in the sample, k_i = the thermal conductivity of sample i, Q_v = the heat loss per unit rod volume due to convection, Q_c = the heat loss per unit rod volume due to conduction and Q_r = the heat loss per unit rod volume due to radiation.

The initial condition is:

$$T = T_o \quad \text{for } -L_2 \leq x \leq L_1 \qquad (2)$$

where L_i = the length of the each sample (i = 1 is the stationary sample and i = 2 is the rotating sample).

The boundary conditions are:

At $x = 0$:

$$-k_1 \frac{\partial T}{\partial x} + k_2 \frac{\partial T}{\partial x} = Q_F \qquad \text{and} \qquad T_{0^+} = T_{0^-} \qquad (3)$$

where Q_F is the total energy flux at the interface via friction and/or reaction.

At $x = L_i$ $(i = 1,2)$:

$$T = T_w = T_o \qquad (4)$$

Energy Flux at the Interface:

In a nonreactive environment the energy flux Q_F is given by the equation

$$Q_F(t) = P(t)v(t)\mu(t) \qquad \text{in Btu/in}^2 \text{ sec.} \qquad (5)$$

The applied pressure (P) and velocity (v) terms are measured quantities but the coefficient of friction (μ) must be determined via a best-fit of the experimental data. For cases where both friction and reaction are important it is possible to simply use the heat flux Q_F as the parameter to be fit. Three correlations are possible for fitting μ or Q_F vs. time:

1. The first model simply states that the parameter to be fit, $p(t)$ (e.g., the heat flux Q_F or friction coefficient μ), will be held constant over a specified time interval Δt_i, i.e.

$$p(t) = p_i \quad \text{for} \quad t_i \leq t \leq t_i + \Delta t_i \qquad (6)$$

2. The second model uses an Nth-degree polynomial to approximate the parameter $p(t)$ via $N+1$ coefficients, i.e.,

$$p(t) = a_0 + a_1 t + a_2 t^2 + \cdots + a_N t^N \qquad (7)$$

3. The third model uses parameters similar to Model 1 but also uses quadratic interpolation to approximate the value of the parameter $p(t)$ as a continuous function of time for all times $t_i \leq t \leq t_i + \Delta t_i$. The parameter values used for interpolation are p_i through p_{i+2}.

Gas-Phase Heat Balance:

For the gas phase the following energy balance was used (assuming the gas phase to be well-mixed):

$$m_g C_{v,g} \frac{dT_g}{dt} = 2\pi R_o \int_{-L_1}^{L_1} h_v (T - T_g) \, dx - A_g h_v (T_g - T_w) \qquad (8)$$

where m_g = the mass of gas in the system, $C_{v,g}$ = the constant volume heat capacity of the gas, h_v = convective heat transfer coefficient, T = the rod temperature (varies with position), T_g = the temperature of the gas, T_w = the chamber wall temperature, R_o = the outer rod radius and A_g = the area for heat transfer from the gas to the surrounding chamber.

Due to the high pressures (above 1,000 psia) used for the oxygen and nitrogen systems, the assumption of ideal gas was inappropriate. This was especially true for physical properties such as heat capacity, thermal conductivity and viscosity. It was therefore decided to use the Lee-Kesler modification of the Benedict-Webb-Rubin equation of state[3] to approximate the departure from the ideal gas properties. (The derivation of the departure equations was carried out by a graduate student (K. Bhattacharrya) under NASA Grant NAG9-557 and will be discussed in more detail in his thesis. It is important to note that the equations for the departure function for gas heat capacity given by both reference 3 and the original paper of Lee and Kesler are incorrect.)

External Heat Transfer From Rods:

The following equations are used for the heat transfer losses from the rods:

Convection: The heat loss from the rods due to convection can be described by the equation

$$Q_v = S_v h_w (T - T_g) \qquad (9)$$

where S_v = the surface area per unit rod volume available for convective heat transfer ($= 2R_o/(R_o^2 - R_i^2)$) and R_i = the inner radius of the annulus. The convective heat transfer coefficient is assumed to be given by a Nusselt number correlation as:

$$Nu = K (Ta/F_g)^a Pr^b \qquad (10)$$

where K, a and b are constants given by one of three methods: 1) the correlation of Becker and Kaye[4], 2) the correlation of Eisenberg et al.[5] or 3) a best-fit of the data. The modified Taylor number is defined as

$$(Ta/F_g) \equiv \frac{\omega^2 R_m d^3}{\nu^2 F_g} \qquad (11)$$

where ω = the angular velocity of the rotating cylinder, $r_m = (R_c + R_o)/2$, $d = R_c - R_o$, R_c = the radius of the chamber, ν = the kinematic viscosity of the gas and F_g = a shape factor given by Becker and Kaye[4].

For heat conduction <u>from</u> the rods to the gas the Nusselt number is defined as

$$Nu \equiv \frac{2h_r R_o}{k_g} \qquad (12)$$

where k_g = the thermal conductivity of the gas. For heat conduction <u>from</u> the gas to the chamber the Nusselt number is defined as

$$Nu \equiv \frac{2h_r R_c}{k_g} \qquad (13)$$

Conduction: For the heat transfer from the cylinders to the holders the heat loss due to conduction is approximated by a "pseudo" heat transfer coefficient h_c

$$Q_c = S_{c,i} h_c (T - T_w) = \frac{S_{c,i} k_g}{\Delta x} (T - T_w) \qquad (14)$$

where $S_{c,i}$ = the surface area per unit volume of rod i available for conductive heat transfer and Δx = the distance separating the cylinder and holder.

Radiation: The heat loss due to radiative heat transfer is calculated via

$$Q_r = S_{r,i} \sigma F_{i-j} (T^4 - T_w^4) \qquad (15)$$

where all temperatures are absolute (°R), σ = Stefan's constant, $S_{r,i}$ = the surface area per unit volume of rod i available for radiative heat transfer and F_{i-j} = the

20-6

shape factor for radiative heat transfer from body *i* to body *j*.

NUMERICAL SOLUTION

The addition of the physical property package for the gases at high pressures resulted in a significant increase in the computation time for the model. It therefore became apparent that a more efficient method for the spatial discretization as well as the time integration would be required to keep the computation times to realistic values.

For the time integration the original subroutine LSODE was replaced by LSODES (which consists of the same integration methods but was designed to more efficiently handle the sparse Jacobian matrices which result from reducing partial differential equations to a series of ordinary differential equations via spatial discretization). LSODES was written by A.C. Hindmarsh and A.H. Sherman. The Runge-Kutta-Fehlberg program RKF45 of H.A. Watts and L.F. Shampine was also included in the program because of its increased robustness. (Both LSODES and RKF45 were obtained through the NETLIB distribution system.)

For the spatial discretization two different methods were incorporated. One method is the same finite difference method as in the original model but, in order to determine the temperatures at the exact axial thermocouple locations, quadratic interpolation was used when these positions were located between grid points. This allowed a significant reduction in the required number of grid points (from 18 to 5) to achieve the same accuracy with respect to measured vs. calculated temperatures.

The second method of spatial discretization was to use orthogonal collocation on finite elements.[6] This method consists of replacing the original partial differential equation with the ordinary differential equation

At $x = x_n$:

$$\frac{dT_n}{dt} = \frac{1}{h^2} \sum_{i=1}^{N+2} A_{ni} k(T_i) \sum_{j=1}^{N+2} A_{ij} T_j - Q_v(T_n) - Q_c(T_n) - Q_r(T_n) \quad (16)$$

where x_n = the nth collocation point in the element, h = the size of the element, A_{ij} = the elements of the $(N+2) \times (N+2)$

matrix approximating the first derivative via orthogonal collocation[6] and N = the number of interior collocation points in each element. Finite elements were used to simplify the integration of the convective heat transfer contribution in the gas energy balance (which was accomplished via quadrature).

Two elements were used in each rod with the boundary of each element being the point where the sample holders ended. The solution at the collocation point at the boundary between the two elements in each sample was handled in the usual way by setting the axial gradients equal to each other. If we number the four elements sequentially with element 1 being the section of the stationary sample in the holder we get the following equation for the boundary of the elements in the stationary sample

$$\frac{1}{L_i - X_e} \sum_{k=1}^{N^{(1)}+2} A_{1,k} T_k^{(1)} = \frac{1}{X_e} \sum_{k=1}^{N^{(1)}+2} A_{N^{(1)}+2,k} T_k^{(2)}$$

where $x_{e,s}$ = the axial position for the location of the boundary between the elements in the stationary sample, $T_i^{(j)}$ = the temperature in element j next at the collocation point i in each element. For the rotating sample we simply replace the superscript (1) with (4) and (2) with (3) and $x_{e,s}$ with $x_{e,r}$, the axial position for the element boundary in the rotating sample.

The boundary condition at the interface was handled in a similar manner

$$-\frac{1}{X_{e,s}} \sum_{k=1}^{N^{(1)}+2} A_{1,k} T_k^{(2)} + \frac{1}{X_{e,r}} \sum_{k=1}^{N+2} A_{1,k} T_k^{(3)} = Q_F$$

To make the program more robust two parameter fitting subroutines have been added. One method is a direct search multivariable simplex method developed by Nelder and Mead.[7] The other subroutine is LMDIF which uses a modification of the Levenburg-Marquardt algorithm and was written by B.S. Grabow, K.E. Hillstrom and J.J. More. (LMDIF was obtained through the NETLIB distribution system.)

Results

The computer program (now called *FHP* and installed on the computer system at WSTF) was tested on five high pressure

systems, all with oxygen at approximately 1,000 psia, and gave the results shown in Table 1. The error in Table 1 refers to the root mean square error between the measured and calculated values for both thermocouples in the stationary sample, 0.05 and 0.20 inches from the interface. Tests 830-198 and 830-199 used AISI 304 stainless steel and tests 830-305 through 830-307 used AISI-316 stainless steel. Physical properties of these materials vs. temperature were obtained from Touloukin.[8]

TABLE 1. RESULTS FOR HIGH-PRESSURE OXYGEN TESTS

Test	Average Error (°F)
830-198	±26.4
830-199	±63.6
830-305	±14.3
830-306	±18.8
830-307	±19.4

The temperatures in the samples varied from initial temperatures of approximately 70 °F to final measured temperatures of from 1,000 to 1,400 °F.

Figure 1 gives an example of the results of using Model 3 to approximate the energy flux at the interface for test 830-307. Thermocouple TC-702 is located 0.05 inches from the interface of the rotating and stationary samples and TC-703 is 0.20 inches away. Also shown is the predicted interface temperature. For the AISI 304 tests (830-198 and 830-199) the calculated temperature drop between TC-702 and TC-703 was significantly smaller than the measured value. This was probably due to inaccurate data for the physical properties of the metals.

Figure 2 shows a comparison of the heat flux (in Btu/in^2sec) at the interface (via Model 3) vs. time (in seconds) for the three repeated tests 830-305, 830-306 and 830-307.

Conclusions

The program *FHP*, developed as a result of the support over the two past summers by the NASA/ASEE Summer Faculty Fellowship

Program, is successful in accurately determining the heat flux and/or friction coefficients necessary to produce the observed temperatures in the WSTF frictional heating apparatus. The program has enough alternatives with respect to spatial discretization, integration and minimization to make it very robust and sufficiently accurate compared to possible inaccuracies in the experiments. The weak points in the program are:

1. The quantitative effects of convection on the heat loss from the samples. At present a simple correlation from studies on annuli with the inner cylinder rotating is used.
2. The physical properties of some of the metals vs. temperature may be inaccurate.
3. The assumption that the holders are at a constant temperature throughout the simulation.
4. The one-dimensional nature of the model.

At present, only the last problem is actively being investigated. As a part of the research under NASA grant NAG9-557 a computer model is being developed in order to determine the possibility of significant radial gradients through the samples for heat fluxes at the interface which vary radially as well as with time. Once this is known a model can then be developed to include angular variations in the heat flux to determine whether there is a significant difference in temperatures at the same axial position but different angular positions.
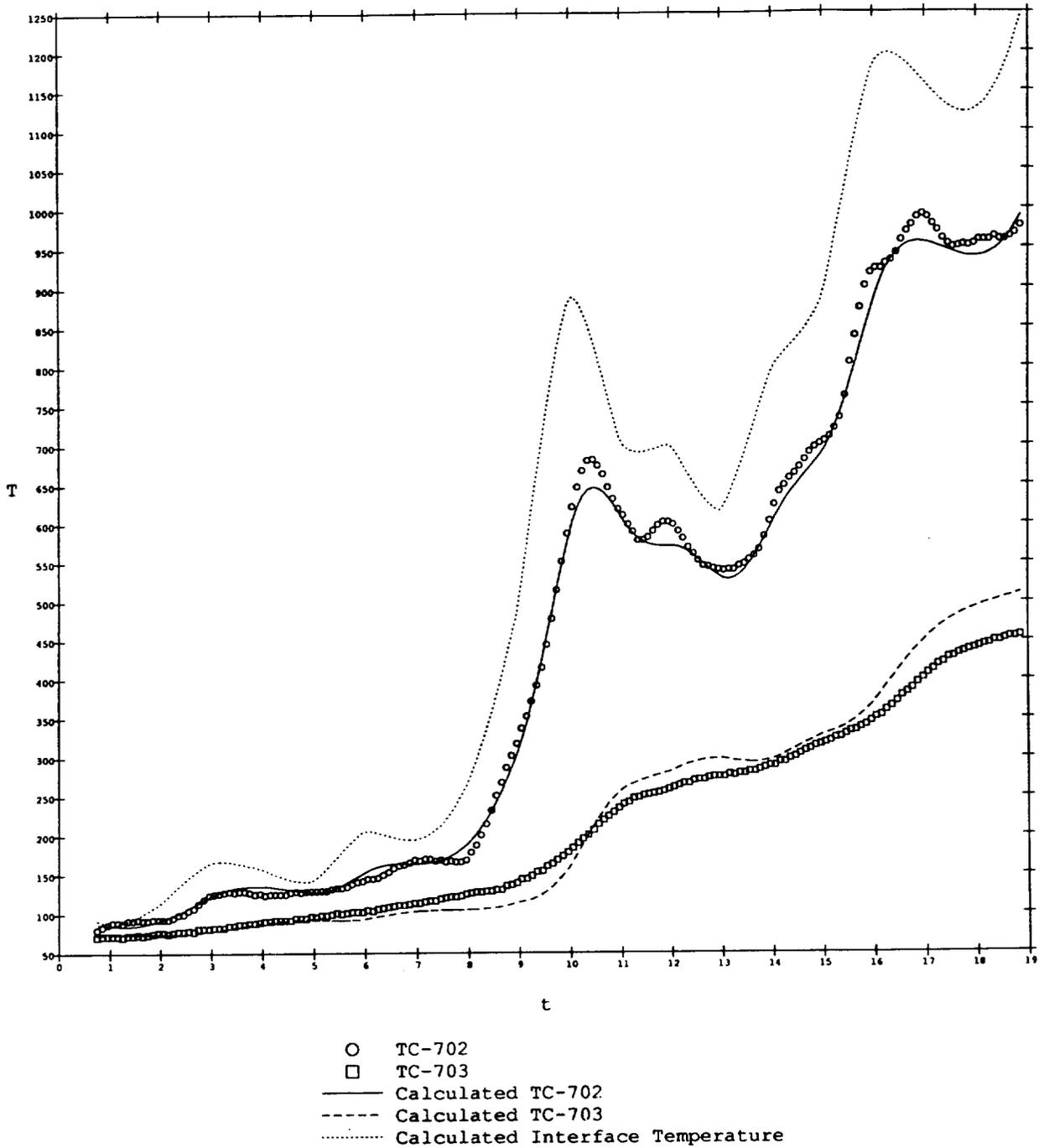
Figure 1. Comparison of measured and calculated temperatures for thermocouples located 0.05 inches (TC-702) and 0.20 inches (TC-703) from the interface. (T in °F and t in sec.)
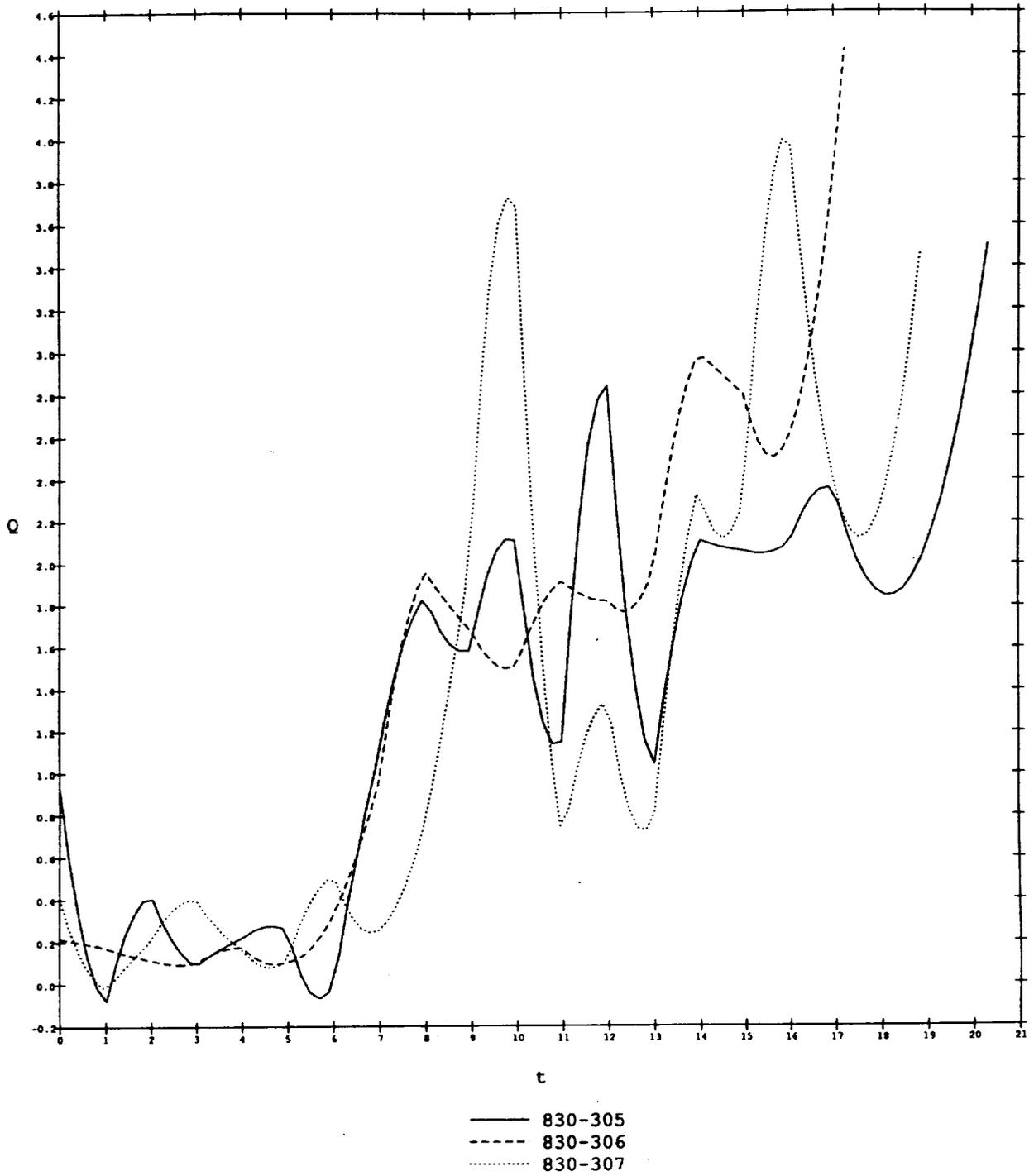
Figure 2. Heat flux at the interface (Q_F in Btu/in^{2}sec.) vs. time (in sec.) for three different tests using Model 3.

REFERENCES

1. Stolzfus, J.M.; Benz, F.J.; and Homa, J.M.: The Pv Product Required for the Frictional Ignition of Alloys. Flammability and Sensitivity of Materials in Oxygen-Enriched Atmospheres: 4th Volume (ASTM STP 1040), J.M. Stolzfus, F.J. Benz and J.S. Stradling, eds., American Society for Testing and Materials (Philadelphia), 1989, pp. 212-223.

2. Skowlund, C.T.; and Beeson, H.D.: Model of the Frictional Heating of Inconel 718 and Titanium (Ti-6V-4Al) in Helium: Final Report for the 1991 NASA/ASEE Summer Faculty Fellowship Program.

3. Reid, R.C.; Prausnitz, J.M.; and Poling, B.E.: The Properties of Gases and Liquids, 4th Edition. McGraw-Hill, 1987.

4. Becker, K.M.; and Kaye, J.: The Influence of a Radial Temperature Gradient on the Instability of Fluid Flow in an Annulus With an Inner Cylinder Rotating. *Transactions of the A.S.M.E., Journal of Heat Transfer*, vol. 84, 1962, pp.106-110.

5. Eisenberg, M.; Tobias, C.W.; and Wilke, C.R.: Mass Transfer at Rotating Cylinders. *Chemical Engineering Progress, Symposium Series No. 16*, vol. 51, 1955, pp.1-16.

6. Finlayson, B.: Nonlinear Analysis in Chemical Engineering. McGraw-Hill, 1980.

7. Nelder, J.A.; and Mead, R.: A Simplex Method for Function Minimization. *Computer Journal*, vol. 7, 1965, pp. 308-313.

8. Touloukin, Y.: Thermophysical Properties of High Temperature Solid Materials: Vol. 3 Ferrous Alloys, The MacMillan Co., 1969.