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ANALYSIS OF REVERSE COMBUSTION IN TAR SANDS:
A ONE-DIMENSIONAL MODEL

By
A. Amr

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University of Wyoming
Laramie, Wyoming 82071

TECHNICAL INFORMATION CENTER
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ABSTRACT

This paper describes a one-dimensional numerical model which simulates oil recovery from tar sands by reverse combustion. The method of lines is used to solve the nonlinear differential equations describing the flow. The effects of volumetric air flux on the peak temperature, flame velocity, and oil recovery efficiency are reported. The results are compared to the results of relevant experimental studies.

NOMENCLATURE

- A_1 = Arrhenius constant for oxygen reaction rate, $\text{kg/m}^3\text{hr}$
 A_2 = Arrhenius constant for pyrolysis rate, $\text{kg/m}^3\text{hr}$
 c = Specific heat, kJ/kg K
 D = Effective diffusion coefficient, m^2/hr
 E_1 = Activation energy for oxygen reaction rate, K
 E_2 = Activation energy for pyrolysis rate, K
 H = Heat released per kg of oxygen consumed, kJ/kg
 K = Effective thermal conductivity, kJ/hr-m K
 m_a = Mass flux of air at inlet, $\text{kg/m}^2\text{hr}$
 m_g = Mass flux of gas, $\text{kg/m}^2\text{hr}$
 M_o = Original bitumen in place, kg/m^3
 N = Weight fraction, nondimensional
 P = Production (pyrolysis) rate of oil $\text{kg/m}^3\text{hr}$
 R = Reaction rate (oxygen), $\text{kg/m}^3\text{hr}$
 t = Time
 T = Temperature, K
 W = Percentage of bitumen in place, nondimensional
 V = Combustion zone velocity, m/hr

Greek Symbols

- ϕ = Porosity, nondimensional
 γ = stoichiometric coefficient, nondimensional
 ρ = density, kg/m^3

Subscripts

- g = gas
 i = i^{th} species (oxygen: $i = 1$, oil: $i = 2$)
 s = solid

I. Introduction

It has been estimated that up to thirty billion barrels of oil are contained in tar sand deposits in five states (California, Kentucky, New Mexico, Texas, and Utah) [1]. The deposits in Utah alone are estimated to contain twenty-eight billion barrels of oil.

The U. S. Department of Energy's (DOE) Laramie Energy Technology Center (LETC) initiated a program in 1971 to develop in situ thermal techniques for recovery of oil from U. S. tar sand deposits. In situ thermal recovery techniques include steam stimulation ("huff and puff"), steam flooding, forward combustion (fire-flooding), reverse combustion, and fire-water flooding (Cofcaw). These techniques have been utilized successfully in enhanced oil recovery and may be suitable for heavy viscous bitumen found in tar sands.

In forward and reverse combustion, air is injected into the formation. The reaction between the oxygen in the air and the coke (in case of forward combustion) and/or a portion of the oil (in case of reverse combustion) produces the heat necessary for viscosity reduction and oil cracking. The air drive produces the necessary pressure gradient to displace the distilled oil and oil vapor, products of combustion, and connate water towards the production well. In forward combustion, the flame front moves in the same direction as the air flow. Oil flow in the colder region ahead of the flame could result in a plugged flow due to the increased oil viscosity in this region. In reverse combustion, such a problem is avoided. The flame front moves in the opposite direction of air flow and oil flows through the heated region towards the production wells.

Theoretical investigations of reverse combustion in tar sands have been relatively scarce. Four major works in this area have been identified; namely, models developed by Berry and Parrish [2], Warren, Reed, and Price [3], Kotowski and Gunn [4], and Land [5]. These models were examined as a starting point for our numerical investigation of reverse combustion in tar sands.

All four models are one-dimensional and assume a quasi-steady state. The latter assumption implies that the temperature and concentration profiles are unchanged with respect to a coordinate system moving with the constant combustion zone velocity. These models solve the energy balance and mass balance equation in order to obtain temperature and concentration profiles together with combustion zone velocity.

The energy equation is given by

$$\frac{d}{dx} K \frac{dT}{dx} - \frac{d}{dx} ((m_g c_g + V(\rho_s c_s + \phi_g \rho_g c_g))T) + \phi_g HR = 0 \quad (1)$$

The conservation of the i^{th} species is given by

$$\frac{d}{dx} \rho D \frac{dN_i}{dx} - \frac{d}{dx} ((m_g + V\phi_g \rho_g)N_i) + P_i - \phi_g \gamma_i R = 0 \quad (2)$$

The dependent variables in equation (1) and (2) are the temperature and the species concentration. All other properties are known except the combustion zone velocity (V). These equations are nonlinear and are coupled through the dependence of the reaction rate on both temperature and concentrations. An additional equation is needed which relates the gas flux with combustion zone velocity and peak temperature. This additional equation is obtained from global heat balance. In such formulation the combustion zone velocity may be considered an eigen-value of the problem.

Berry and Parrish [2] and Land [5] neglected the diffusion term in equation (2) and considered only the oxygen balance. Furthermore, they assumed a reaction rate which is independent of oxygen concentration. The latter assumption decouples equation (1) from equation (2). Berry and Parrish added a heat loss term to the energy equation.

Warren et. al. [3] included the diffusion term in their model and examined the dependence of the reaction rate on oxygen concentration. All three investigators assumed constant physical properties.

The above mentioned models could be used to estimate the effects of air flux on both the combustion zone velocity and the peak temperature. These results are found to agree satisfactorily with the results of adiabatic tube runs. These models, however, cannot predict either the oil production rate or recovery efficiency. This is because none of the models included an oil mass balance in their analysis.

The model of Kotowski and Gunn was developed to examine the underground coal gasification process. This model is by far the most general of the four available models and includes the effects of variation of physical properties with temperature. It also solves a fuel mass balance in addition to the oxygen balance and energy balance. The Kotowski-Gunn Model predicts the gas production rate, peak temperature, and combustion zone velocity.

II. Mathematical Model

A one-dimensional unsteady state model, which simulates reverse combustion in tar sands, is described in this section. The model simulates a reverse combustion experiment similar to the tube runs described by Land [6] and Reed et.al. [7]. In such experiments, a tube

was packed with tar sands and was heated at one end while air was injected at a constant flow rate at the other end. When ignition was initiated, heating was stopped and a flame front propagating downstream was observed. Heat losses during the run were prevented by the use of perimeter heating to reduce temperature gradients in the radial direction. A model which describes such experiments consists of a system of four coupled partial differential equations which result from energy and mass conservation laws and kinetic data. These equations are summarized below.

Energy Equation

$$(\rho_s c_s + \phi_g \rho_g c_g) \frac{\partial T}{\partial t} = K \frac{\partial^2 T}{\partial x^2} - m_g c_g \frac{\partial T}{\partial x} + \phi_g HR \quad (3)$$

Oxygen Concentration Equation

$$\phi_g \rho_g \frac{\partial N_1}{\partial t} = - m_g \frac{\partial N_1}{\partial x} - \phi_g R - N_1 P \quad (4)$$

Oil Vapor Concentration Equation

$$\phi_g \rho_g \frac{\partial N_2}{\partial t} = - m_g \frac{\partial N_2}{\partial x} - \gamma \phi_g R + P(1 - N_2) \quad (5)$$

Oil Pyrolysis Rate

$$M_o \frac{dW}{dt} = P \quad (6)$$

The subscripts 1 and 2 refer to oxygen and oil respectively.

In deriving the above equations, the following assumptions have been made.

- (1) Porosity, specific heats of solid and gas, thermal conductivity of tar sands, and heat of reaction are assumed constant and uniform.
- (2) The gas and solid temperatures are equal.

- (3) Heat losses and molecular diffusion were not considered. In a more comprehensive model, these effects may be easily incorporated.

Arrhenius type expressions for the oxygen reaction rate (R) and the oil pyrolysis rate (P) were obtained from references [5] and [8] respectively.

Thus:

$$R = A_1 \text{EXP} (-E_1/T) \quad (7)$$

$$P = A_2 \text{EXP} (-E_2/T) \quad (8)$$

In order to solve the system of equations (3) through (6) (i.e., to obtain the values of T, N_1 , N_2 , and W as functions of time and space), the values of physical and chemical properties which appear in these equations should be available to the user. A summary of the values used to test the model are found in Table I. In addition, the following expression for the gas flux m_g was used.

$$m_g = m_a + \int_0^x P \, dx \quad (9)$$

Equation (9) accounts for the change of gas flux as a result of oil production by pyrolysis.

The initial and boundary conditions for this problem are given by:

at $t = 0$ and all x ,

$$T = 294^\circ\text{K}, N_1 = .23, N_2 = 0 \quad (10)$$

at $x = 0$ and all t ,

$$T = 294^\circ\text{K}, N_1 = .23, N_2 = 0 \quad (11)$$

at $x = L$ and $t < \frac{1}{2}$ hour,

$$T = 755.5^\circ\text{K} \quad (12)$$

at $x = L$ and $t > \frac{1}{2}$ hour,

$$\frac{dT}{dx} = 0 \quad (13)$$

III. Numerical Studies

The rate equations (7) and (8) with the gas flux equation (9) were substituted into the system of partial differential equations (3) through (6). The physical and chemical properties, summarized in Table I, were incorporated with equations (3) through (6) and the resulting system was solved by the method of lines [9]. In this method, the tube is divided into equidistant nodal points. The spatial derivatives in the right hand side of equations (3) through (6) are discretized by a standard finite difference technique, while the temporal partial derivative in the left hand side is replaced by a total derivative. If this procedure is carried out for each nodal point, one obtains a system of ordinary differential equations to be integrated numerically. After each integration step, the gas flux and oil produced are calculated.

Due to the hyperbolic nature of equations (4) and (5), the choice of a finite difference approximation is of utmost importance. In this problem, backward difference approximation is recommended. Other approximations, such as centered difference, will lead to instability.

The choice of ordinary differential equation integration technique is also of utmost importance. For example, the standard Adams or Runge-Kutta integrating methods are unstable in connection with this "stiff" system of ordinary differential equations. This phenomenon has been observed with problems involving fast reaction rates. Instead, the more powerful backward differentiation techniques need to be used[10].

The basic advantage of the method of lines in connection with partial differential equations over finite difference techniques is that at each time step the calculation procedure gives an estimate for the local truncation error. Thus one can change the time step size if the truncation error exceeds a preselected value. In finite difference techniques, such

a control of time step size is absent and an ad hoc trial and error procedure is necessary in order to select a time step size. Another advantage of the method of lines over finite difference techniques is that the computer program can be easily written and modified, especially when one is dealing with nonlinear equations.

IV. Results and Conclusions

Six computer runs were completed for six different volumetric air fluxes (namely 3.05, 6.10, 9.14, 12.14, 15.24, 18.29 standard $\text{m}^3/\text{hr-m}^2$, which correspond to 10, 20, 30, 40, 50 and 60 ft/hr respectively). As air flux increased and temperature and concentration gradients became steeper, instability occurred with improper choice of time and length steps.

After the completion of each run, the following results are obtained at hourly intervals:

- (1) Temperature profile
- (2) Oxygen concentration profile as a fraction of the original oxygen concentration
- (3) Oil concentration profile as a fraction of gas density
- (4) The oil accumulated

Figures 1, 2, and 3 illustrate the temperature, oxygen concentration and oil concentration profiles, respectively, at two hour intervals, for an air flux of 9.14 standard $\text{m}^3/\text{hr-m}^2$. It can be seen that steady state conditions were achieved within six hours. The other computer runs indicate that as the air flux is reduced below 9.14 $\text{m}^3/\text{hr-m}^2$, steady state conditions are not attained. It can be deduced from this that the steady state analysis presented in the introduction is only valid for air fluxes in excess of 9.14 standard $\text{m}^3/\text{hr-m}^2$, and that the stabilization time in such cases is on the order of two hours.

In Figures 4 and 5, the effect of air flux on the peak temperature and flame velocity are presented respectively. In Figure 6, oil recovery efficiency is plotted versus air flux. Here the recovery efficiency is defined as the fraction of original oil in place which was produced by the reverse combustion techniques. It is to be noted from Figure 6 that for air fluxes in excess of 12 standard $\text{m}^3/\text{m}^2\text{hr}$, no appreciable increase of oil recovery efficiency is observed. This may be explained as follows: As air flux increases, the peak temperature increases, and this increases both the oxygen reaction rate and oil pyrolysis rate. Thus, as temperature increases, more oil is pyrolyzed, but also more oil reacts with oxygen. Experimental results by Land [5] indicate that oil recovery decreases slightly for air flux of 18 standard $\text{m}^3/\text{m}^2\text{hr}$.

The results shown in figures 4 and 6 were compared with the experimental results of Land [6] and were found to be in satisfactory agreement as shown in Table II. The discrepancy between the experimental and numerical values may be attributed to the uncertainty in the physical and chemical properties outlined in Table I. The fact that the temperatures attained in the numerical runs are consistently higher than the corresponding experimental values indicates that the adiabatic conditions assumed here are too stringent.

Finally, the results here are important for the study of the effects of various parameters on the recovery efficiency and illustrate the viability of the method of lines for such a study. However, the technique presented here becomes more important if two- or three-dimensional flows are considered. In such circumstances, steady state analysis becomes very difficult; and short of an expensive field experiment, the only methods available to us are numerical techniques such as presented here.

V. Acknowledgments

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Table I

Physical and Chemical Data

c_g	= 1.03	kJ/kg K
$c_s \rho_s$	= 2346.88	kJ/m ³ K
ϕ	= 0.26	Dimensionless
K	= 5.3	kJ/hr-m K
ρ_g	= 1.027	kg/m ³
A_1	= 31.395×10^6	kg of oxygen/m ³ hr
E_1	= 6944.44	K
H	= 12,908.4	kJ/kg of oxygen
A_2	= 5.94×10^{10}	hr ⁻¹
E_2	= 16,666.67	K
M_o	= 160.18	kg of oil/m ³

Table II
Comparison Between Numerical Results
and Experimental Results of Reference [5]

Air Flux $\text{cm/m}^2\text{hr}$	Maximum Temperature (K)		Recovery Efficiency (%)	
	Experimental	Numerical	Experimental	Numerical
6.10	610.00	637.90	29.0	14.4
9.14	658.90	683.17	40.8	30
12.19	713.89	722.61	43.5	40
15.24	728.89	756.03	49.6	41.5
18.29	756.10	785.48	40.5	44

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CAPTIONS FOR FIGURES THAT FOLLOW

Figure 1: Temperature profiles at two-hour intervals along the tube length

Figure 2: Oxygen concentration profile as a fraction of original oxygen mass fraction at two-hour intervals along the tube length

Figure 3: Oil concentration as a fraction of mass flux at two-hour intervals along the tube length

Figure 4: Peak temperature versus volumetric air flux

Figure 5: Flame velocity versus volumetric air flux

Figure 6: Oil recovery efficiency versus volumetric air flux

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

APPENDIX A

One Dimensional Reverse Combustion Program "COMBU"

Description of the Computer Program "COMBU"

The computer program "COMBU" developed under this contract solves equations (3) through (6), subject to the boundary and initial conditions outlined above. The version of COMBU described in this appendix and which is listed in Appendix B, is based on the English System of units. Minor modifications of the program are needed to convert to the international system of units.

An automatic ordinary differential equation integrator developed at the Lawrence Livermore Laboratory under the code name GEARB must be used together with COMBU. For a detailed description of GEARB the reader is referred to an article by Hindmarsh [10].

The computer program COMBU consists of four segments; the main program, subroutine DIFFUN, subroutine PDTP, and subroutine DRIVEB.

In the main program, the coefficients needed in equations (3) through (6) are calculated and the initial conditions are formulated. Subsequently, the main program functions as a driver for the integration processes. Finally, program output is handled in this segment. The subroutine DIFFUN provides the system of ordinary differential equations, together with the boundary conditions required by the method of lines. The subroutine PDP calculates the Jacobian for these ordinary differential equations. The Jacobian is required in the backward differentiation techniques. Finally, the subroutine DRIVEB is the automatic differential equations integrator referred to above by GEARB.

A-Input Data

Physical and chemical data pertaining to the problem should be provided by the user. In all, nineteen constants are needed, eleven of which

were described in Table I. All input data require nineteen input cards read by FORMAT (F 19.6). The contents of these cards are described below. It is to be noted that the English System of units has been included in this version.

Card 1 - Contain CG = specific heat of produced gas in Btu/lb°F (e.g. = .245).

Card 2 - Contains PHIG = porosity, non-dimensional (e.g. = .26).

Card 3 - Contains GAMAMC = heat capacity per unit matrix volume in Btu/ft³°F (e.g. = 35)

Card 4 - Contains AH = heating value of oil in But/lb (e.g. = 5550).

Card 5 - Contains CO = original oxygen mass fraction in air, non-dimensional (e.g. = .23).

Card 6 - Contains GAMAG = average produced gas density in lb/ft³ or from ideal gas formula: density = GAMAG/(temp °R) (e.g. = 115.3).

Card 7 - Contains AK = thermal conductivity of solid matrix in Btu/hrFt°F (e.g. = .85).

Card 8 - Contains U = standard air flux in SCF/ft²hr at 1 atm and 60°F (treated as a parameter).

Card 9 - Contains E = activation energy for oxygen-oil reaction °R (e.g. = 12,500).

Card 10 - Contains A = Arrhenius constant for oxygen-oil reaction in lb of oxygen/ft³-hr (e.g. = 1.96×10^6).

Card 11 - Contains E2 = activation energy for oil pyrolysis in °R (e.g. = 30,000).

Card 12 - Contains A2 = Arrhenium constant for oil pyrolysis in hr⁻¹ (e.g. = 5.94×10^{10}).

Card 13 - Contains GAMAG2 = air density under standard conditions in lb/ft^3 (e.g. = .076).

Card 14 - Contains BETA = mass of oil reacted per mass of air, non-dimensional (e.g. = 0.541).

Card 15 - Contains OILM = lbs of oil available for combustion and/or production per cubic foot of solid matrix (a variable which depends on temperature, and considered constant for each run) (e.g. = 10).

Card 16 - Contains FEET = length of combustion tube in feet (e.g. = 4).

Card 17 - Contains TMAX = time at which integration stops, in hours (e.g. = 30).

Card 18 - Contains DTHET = time step, in hours, a value less than 2.5×10^{-3} is recommended.

Card 19 - Contains W11 = time of heating the tube end at exit, in hours (e.g. = .5 for $U \leq 30$ and = 1 for $U > 30$).

B-Program Output

The reader is referred to Appendix C for a sample printout.

1. The program lists all nineteen input values by the designation described above. In addition, the length increment DX and the number of equation to integrated NFUNCT are listed.
2. The results at each time step are preceded by numbers. The first number is the last time step used. The second number is an index for the integration procedure (usually equal to two except for the first step where it is equal to one); the third number is NFUNCT, the number of equation to be integrated. Finally, the last number is the current time in hours, for which the results are listed.

3. Under the heading, "TEMPERATURE," the values of the temperature at the current time are listed for each mesh point starting from the inlet end.
4. Under the heading, "OXYGEN CONCENTRATION," the values of oxygen concentration as a percentage of the original oxygen concentration at inlet, are listed for each mesh point. A value of one under this heading indicates no reaction with oxygen did occur.
5. Under the heading, "OIL CONCENTRATION," the values of oil vapor concentration in the gas stream (lb of oil per lb of gas mixture) are listed for each point.
6. Under the heading, "JWW," the values of the fraction of oil in place, which is pyrolyzed, are listed. A value of one means that only coke is left in place.
7. The mass flow rate per unit area at exit, "LAST DOTM", and the mass of oil collected up to this time, "SUMOIL," are listed.
8. The results are printed at hourly intervals in the format described in item 2 through 7.

C-Notes on the Use of the Program

1. The program uses eighty mesh points; if fewer points are desired, the user has to change card number 26 in the main program so that JJBED = number of mesh points. If more than eighty points are required, in addition to the above change, the user has to change three "DIMENSION" statements; one in the main program, and one each in subroutine DIFFUN and PDP, such that the statements read:

DIMENSION DOTM(JJBED), P(4*JJBED), DERYL(4*JJBED)

where:

JJBED is the new number of mesh points.

2. It is to be noted that a portion of the Bitumen in the tar sands converts to coke which is not available for combustion. The amount of coke formed is a strong function of temperature. The value of OILM described in the input data, card 15, is the difference between the oil in place and the coke formed. Thus OILM is also a function of temperature and thus is not known at the beginning of the computer run. To avoid this difficulty, the following procedure is suggested:

A preliminary run is conducted with OILM taken as the oil in place up to time equal to five hours. This run will determine the temperature profile which is insensitive to the value of OILM. Once the maximum temperature is known for a given air flux, a more realistic OILM can be estimated. Namely, experimental data are available which relate OILM as a function of temperature [7].

3. A complete run requires between 20 to 50 minutes of computer time using the University SIGMA 7 computer.

APPENDIX B

Listing of Program COMBU

```

C*****
C
C   THIS IS THE OCTOBER 1979 VERSION OF:
C   COMBU, A ONE-DIMENSIONAL REVERSE COMBUSTION MODEL.
C
C   INPUT PARAMETERS:
C       CG      = SPECIFIC HEAT OF GAS
C       PHIG     = POROSITY
C       GAMAMC   = HEAT CAPACITY PER UNIT MATRIX VOLUME
C       AH       = HEATING VALUE OF OIL
C       C0       = ORIGINAL OXYGEN MASS FRACTION IN AIR
C       GAMAG    = AVERAGE GAS DENSITY
C       AK       = THERMAL CONDUCTIVITY OF SOLID MATRIX
C       U        = STANDARD AIR FLUX
C       E        = ACTIVATION ENERGY FOR OXYGEN-OIL REACTION
C       A        = ARRHENIUS CONSTANT FOR OXYGEN-OIL REACTION
C       E2       = ACTIVATION ENERGY FOR OIL PYROLYSIS
C       A2       = ARRHENIUS CONSTANT FOR OIL PYROLYSIS
C       GAMAG2   = AIR DENSITY UNDER STANDARD CONDITIONS
C       BETA     = MASS OF OIL REACTED PER MASS OF AIR
C       OILM     = LBS OF OIL AVAILABLE FOR COMBUSTION AND PRO-
C                   Duction PER CUBIC FOOT OF SOLID MATRIX
C       FEET     = LENGTH OF COMBUSTION TUBE
C       TMAX     = TIME AT WHICH INTEGRATION STOPS
C       DTHET    = TIME STEP, RECOMMENDED LESS THAN 2.5 * 10**-3
C       W11     = TIME OF HEATING TUBE END AT EXIT
C
C*****
C   DIMENSION DOTM(80), P(320)
C   COMMON W0, W1, W2, W3, W4, W5, W6, W7, W8, W11, A2, OILM,
C           DOTM, DTHET, DX, E, E2, JJBED
C   READ(5,100) CG, PHIG, GAMAMC, AH, C0, GAMAG, AK, U, E, A, E2,
C           A2, GAMAG2, BETA, OILM, FEET, TMAX, DTHET, W11
C   JJBED = 80
C   N     = 4 * JJBED
C   DX    = FEET / (JJBED - 1.0)
C   WRITE(3,110) CG, PHIG, GAMAMC, AH, C0, GAMAG, AK, U, E, A, E2,
C           A2, GAMAG2, BETA, OILM, FEET, TMAX, DTHET, W11, DX, N
C*****
C
C   VARIABLE INITIALIZATION.
C
C*****
C       W0 = - BETA * A / GAMAG
C       W1 = AK / DX**2 / (GAMAG2 * PHIG * CG + GAMAMC)
C       W2 = - CG / (2.0 * DX) / (GAMAG2 * PHIG * CG + GAMAMC)
C       W3 = (PHIG * AH * A) / (GAMAG2 * PHIG * CG + GAMAMC)
C       W4 = - 1.0 / (GAMAG * PHIG * DX)
C       W5 = - A / (C0 * GAMAG)
C       W6 = - (OILM * A2) / (GAMAG * PHIG)
C       W7 = OILM * A2
C       W8 = - GAMAG * PHIG
C       T0 = 0.0
C       H0 = DTHFT
C       MF = 21
C       ML = 4
C       MU = 4
C       EPS = 0.01
C       TOUT = 0.0
C       KCNT = 100

```

```

INDEX = 1
SUMOIL = 0.0

C
XTEMP = GAMAG2 * U
DO 10 J = 1,N-3,4
  P(J) = 70.0
  P(J+1) = 1.0
  P(J+2) = 0.0
  P(J+3) = 0.0
10 DOTM((J+3)/4) = XTEMP
C
P(N-3) = 900.0
P(N-2) = 1.0
P(N-1) = (OILM * DX) / (OILM * DX + 2.0 * XTEMP)
P(N) = 1.0
GO TO 40

C*****
C
C CALL DRIVEB TO INTEGRATE THE SYSTEM *
C OF FOUR O.D.E.'S AT TIME = TOUT. *
C *
C*****
20 CALL DRIVEB(N,T0,H0,P,TOUT,EPS,MF,INDEX,ML,MU)
INDEX = 2
DOTM(2) = DOTM(1) + ( 1.0 - P(4) ) * W7 * DX *
  DEXP( -E2 / ( P(1) + 460.0 ) ) / 2.0
DO 30 J = 3,JJBED
  WJ = 1.0 - P(J*4-4)
  RP = W7 * WJ * DEXP( -E2 / ( P(J*4-7) + 460.0 ) )
  P2 = WJ * OILM / DTHET
  IF (RP .GT. P2) RP = P2
30 DOTM(J) = RP * DX + DOTM(J-1)
SUMOIL = SUMOIL + DOTM(JJBED) * P(N-1) * DTHET
C*****
C
C OUTPUT EVERY 100TH SOLUTION. *
C *
C*****
40 IF (KCNT .LT. 100) GO TO 50
KCNT = 0
WRITE(3,120) H0, INDEX, N, TOUT
WRITE(3,130)
WRITE(3,140) (P(J), J = 1,N-3,4)
WRITE(3,150)
WRITE(3,140) (P(J), J = 2,N-2,4)
WRITE(3,160)
WRITE(3,140) (P(J), J = 3,N-1,4)
WRITE(3,170)
WRITE(3,140) (P(J), J = 4,N,4)
WRITE(3,180) DOTM(JJBED), SUMOIL
50 KCNT = KCNT + 1
TOUT = TOUT + DTHET
IF (TOUT .LE. TMAX) GO TO 20
C*****
C
C PROGRAM EXIT. *
C *
C*****
WRITE(3,190) H0, INDEX, N, TOUT, SUMOIL
STOP

```

```

C
100 FORMAT(18(F19.6,/),F19.6)
110 FORMAT('CG      ='F19.6/'PHIG  ='F19.6/'GAMAMC='F19.6/
1      'AH      ='F19.6/'C0    ='F19.6/'GAMAG  ='F19.6/
2      'AK      ='F19.6/'U      ='F19.6/'E       ='F19.6/
3      'A       ='F19.6/'E2     ='F19.6/'A2      ='F19.6/
4      'GAMAG2='F19.6/'BETA   ='F19.6/'OILM   ='F19.6/
5      'FEET    ='F19.6/'TMAX  ='F19.6/'DTHET  ='F19.6/
6      'W11     ='F19.6/'DX    ='F19.6/'NFUNCT='I6)
120 FORMAT(////////'*****'F13.9,2I6,F13.9/)
130 FORMAT(1X,'TEMPERATURE')
140 FORMAT(1X,10F12.6)
150 FORMAT(1X,'OXYGEN CONCENTRATION')
160 FORMAT(1X,'OIL CONCENTRATION')
170 FORMAT(1X,'JWW')
180 FORMAT(' LAST DOTM ---- 'F13.9/' SUMOIL  ---- 'F13.9)
190 FORMAT(////' *DONE*'F13.9,2I6,F13.9/' SUMOIL ---- 'F13.9)
END
C*****
C
C      DIFFUN COMPUTES:  DERY1 = F(P,T), THE RIGHT SIDE OF THE
C                        O.D.E. INPUT TO DRIVED FOR SOLUTION.
C                        P AND DERY1 ARE VECTORS OF LENGTH N.
C                        THIS ROUTINE IS CALLED BY DRIVED.
C*****
C
C      SUBROUTINE DIFFUN(N,T,P,DERY1)
C      DIMENSION DOTM(80), P(320), DERY1(320)
C      COMMON W0, W1, W2, W3, W4, W5, W6, W7, W8, W11, A2, OILM,
C      DOTM, DTHET, DX, E, E2, JJBED
C*****
C
C      DERIVATIVES AT LOWER BOUNDARY.
C*****
C
C      IF ( P(2) .LT. 0.0 ) P(2) = 0.0
C      IF ( P(3) .LT. 0.0 ) P(3) = 0.0
C      IF ( P(4) .GT. 1.0 ) P(4) = 1.0
C
C      TT = P(1) + 460.0
C      XX = P(2) * DEXP(-E / TT)
C      RP = W7 * ( 1.0 - P(4) ) * DEXP(-E2 / TT)
C      YY = RP / W8
C
C      DERY1(1) = 2.0 * W1 * ( P(5) - P(1) ) + W3 * XX
C      DERY1(2) = 0.0
C      DERY1(3) = (W0 * XX + P(3) * YY - YY) * TT
C      DERY1(4) = RP / OILM
C*****
C
C      NON-BOUNDARY DERIVATIVES.
C*****
C
C      DO 500 JT = 5,N-7,4
C      JC = JT + 1
C      JF = JT + 2
C      JW = JT + 3
C      I = (JT + 3) / 4
C
C      IF ( P(JC) .LT. 0.0 ) P(JC) = 0.0

```



```

      IF ( P(JF) .LT. 0.0 )   P(JF) = 0.0
      IF ( P(JW) .GT. 1.0 )   P(JW) = 1.0

C
      T0 = P(JT)
      TT = T0 + 460.0
      TM = P(JT-4)
      TP = P(JT+4)
      CC = P(JC)
      CM = P(JC-4)
      CP = P(JC+4)
      FF = P(JF)
      FM = P(JF-4)
      FP = P(JF+4)
      WW = P(JW)
      WM = P(JW-4)
      WP = P(JW+4)
      SS = 1.0 - WW

C
      DOTM(I) = DOTM(I-1) + RP * DX
      IF ( I .EQ. 2 )   DOTM(2) = DOTM(1) + RP * DX / 2.0
      DT = DOTM(I)
      XX = CC * DEXP(-E / TT)
      RP = W7 * SS * DEXP(-E2 / TT)

C
      IF ( T .LT. 3.0 )   GO TO 400
      IF ( WM .GE. 1.0 .AND. WP .GE. 1.0 )   GO TO 300
      IF ( T0 .LT. 200.0 )   GO TO 200
C*****
C
C      FIND AVERAGE WEIGHTED VALUES FOR RP AND XX.
C
C*****
      X = ( ( 3.0 * T0 + TM ) / 4.0 ) + 460.0
      Y = ( 3.0 * WW + WM ) / 4.0
      Z = ( 3.0 * CC + CM ) / 4.0
      RP1 = ( 1.0 - Y ) * DEXP(-E2 / X)
      XX1 = Z * DEXP(-E / X)

C
      X = ( ( 3.0 * T0 + TP ) / 4.0 ) + 460.0
      Y = ( 3.0 * WW + WP ) / 4.0
      Z = ( 3.0 * CC + CP ) / 4.0
      RP2 = ( 1.0 - Y ) * DEXP(-E2 / X)
      XX2 = Z * DEXP(-E / X)

C
      RP = W7 * ( RP1 + RP2 ) / 2.0
      XX = ( XX1 + XX2 ) / 2.0
      GO TO 400
C*****
C
C      NO AVERAGING.
C
C*****
200      XX = 0.0
300      RP = 0.0
400      P2 = OILM * SS / DTHET
      IF ( RP .GT. P2 )   RP = P2
      YY = RP / W8

C
      DERY1(JT) = W1 * ( TP + TM - T0 * 2.0 )
               + W2 * ( TP - TM ) * DT + W3 * XX

```

```

DERY1(JC) = (W4 * (CC - CM) * DT + W5 * XX + CC * YY) * TT
DERY1(JF) = (W4 * (FF - FM) * DT + W0 * XX + FF * YY - YY) * TT
500 DERY1(JW) = RP / OILM
C*****
C
C DERIVATIVES AT UPPER BOUNDARY.
C
C*****
C
IF ( P(N-2) .LT. 0.0 ) P(N-2) = 0.0
IF ( P(N-1) .LT. 0.0 ) P(N-1) = 0.0
IF ( P(N) .GT. 1.0 ) P(N) = 1.0
C
TT = P(N-3) + 460.0
XX = P(N-2) * DEXP(-E / TT)
DOTM(JJBED) = DOTM(JJBED-1) + RP * DX
C
DERY1(N-2) = (W4 * (P(N-2) - P(N-6)) * DOTM(JJBED) + W5 * XX) * TT
DERY1(N-3) = 0.0
IF (T .LT. W11) GO TO 600
DERY1(N-3) = 2.0 * W1 * (P(N-7) - P(N-3)) + W3 * XX
600 DERY1(N-1) = (W4 * (P(N-1) - P(N-5)) * DOTM(JJBED) + W0 * XX) * TT
DERY1(N) = 0.0
C
RETURN
END
C*****
C
C PDB COMPUTES: THE N BY N JACOBIAN MATRIX OF PARTIAL
C DERIVATIVES, AND STORES IT IN PD AS AN
C N0 BY ML+MU+1 ARRAY. PD(I,J-I+ML+1) IS
C SET TO THE PARTIAL DERIVATIVE OF PDOT
C WITH RESPECT TO P(J). THIS ROUTINE IS
C CALLED BY DRIVED.
C
C*****
C
SUBROUTINE PDB(N,T,P,PD,N0,ML,MU)
DIMENSION DOTM(80), P(320), PD(320,9)
COMMON W0, W1, W2, W3, W4, W5, W6, W7, W8, W11, A2, OILM,
DOTM, DTHET, DX, E, E2, JJBED
C*****
C
C ALL PARTIALS = 0 UNLESS CHANGED BELOW.
C
C*****
C
DO 100 J = 1,N
DO 100 I = 1,9
100 PD(J,I) = 0.0
C*****
C
C PARTIALS AT LOWER BOUNDARY.
C
C*****
C
TT = P(1) + 460.0
CC = P(2)
FF = 1.0 - P(3)
WJ = 1.0 - P(4)
Y = DEXP(-E / TT)
Z = DEXP(-E2 / TT)
YT = Y * (E / TT**2)
ZT = Z * (E2 / TT**2)

```

```

C
PD(1,5) = - 2.0 * W1 + W3 * CC * YT
PD(1,6) = W3 * Y
PD(1,9) = 2.0 * W1
PD(3,3) = (W0 * YT * CC - W6 * WJ * ZT * FF) * TT
          + W0 * Y * CC - W6 * WJ * Z * FF
PD(3,4) = W0 * Y * TT
PD(3,5) = W6 * WJ * Z * TT
PD(3,6) = W6 * FF * Z * TT
PD(4,2) = A2 * ZT * WJ
PD(4,5) = - A2 * Z
C*****
C                                     *
C   NON-BOUNDARY PARTIALS.           *
C                                     *
C*****
DO 200 JT = 5,N-7,4
  JC = JT + 1
  JF = JT + 2
  JW = JT + 3
  DT = DOTM((JT+3)/4)
  TT = P(JT) + 460.0
  CC = P(JC)
  CM = P(JC-4)
  FF = 1.0 - P(JF)
  WJ = 1.0 - P(JW)
  Y = DEXP(-E / TT)
  Z = DEXP(-E2 / TT)
  RP = W7 * Z * WJ
  P2 = OILM * WJ / DTHET
  IF (RP .GT. P2) Z = 1.0 / (A2 * DTHET)
  YT = Y * (E / TT**2)
  ZT = Z * (E2 / TT**2)
C
PD(JT,1) = W1 - W2 * DT
PD(JT,5) = - 2.0 * W1 + W3 * CC * YT
PD(JT,6) = W3 * Y
PD(JT,9) = W1 + W2 * DT
C
PD(JC,1) = - W4 * DT * TT
PD(JC,4) = (W5 * CC * YT + W6 * WJ * ZT * CC) * TT
          + W4 * (CC - CM) * DT + W5 * CC * Y + CC * RP / W8
PD(JC,5) = (W4 * DT + W5 * Y + W6 * Z * WJ) * TT
PD(JC,7) = - W6 * CC * Z * TT
C
PD(JF,1) = - W4 * DT * TT
PD(JF,3) = (W0 * YT * CC - W6 * WJ * ZT * FF) * TT
          + W0 * Y * CC - W6 * WJ * Z * FF
PD(JF,4) = W0 * Y * TT
PD(JF,5) = (W4 * DT + W6 * WJ * Z) * TT
PD(JF,6) = W6 * Z * FF * TT
C
PD(JW,2) = A2 * ZT * WJ
PD(JW,5) = - A2 * Z
200 CONTINUE
C*****
C                                     *
C   PARTIALS AT UPPER BOUNDARY.      *
C                                     *
C*****

```

```

DT = DOTM(JJBED)
TT = P(N-3) + 460.0
CC = P(N-2)
CM = P(N-6)
X = DEXP(-E / TT)
XT = X * (E / TT**2)

```

C

```

PD(N-1,1) = - W4 * DT * TT
PD(N-1,3) = W0 * XT * CC * TT + W4 * (P(N-1) - P(N-5)) * DT
PD(N-1,4) = W0 * X
PD(N-1,5) = W4 * DT * TT

```

C

```

PD(N-2,1) = - W4 * DT * TT
PD(N-2,4) = W5 * XT * CC + (W4 * (CC - CM) * DT + W5 * CC * X) * TT
PD(N-2,5) = (W5 * X + W4 * DT) * TT

```

C

```

IF (T .LT. W11) RETURN

```

C

```

PD(N-3,1) = 2.0 * W1
PD(N-3,5) = - 2.0 * W1 + W3 * XT * CC
PD(N-3,6) = W3 * X

```

C

```

RETURN
END

```

APPENDIX C

A Sample Computer Printout

CG	=	.245000
PHIG	=	.260000
GAMAMC	=	35.000000
AH	=	5550.000000
C0	=	.233000
GAMAG	=	115.330000
AK	=	.850000
U	=	30.000000
E	=	12500.000000
A	=	1960000.000000
E2	=	30000.000000
A2	=	59400000000.000000
GAMAG2	=	.076900
BETA	=	.541000
OILM	=	5.500000
FEET	=	4.000000
TMAX	=	20.000000
DTHET	=	.100000
W11	=	1.000000
DX	=	.050633
NFUNCT	=	320

TEMPERATURE

[illegible]

OXYGEN CONCENTRATION

[illegible]

OIL CONCENTRATION

[illegible]

لغات

[illegible]

```

LAST DOTM ---- 2.3070000000
SUMOIL ---- .0000000000

```

*00000000 .013533437 2 320 10.000000000

TEMPERATURE

70.016419	70.016186	70.015968	70.015765	70.015578	70.015409	70.015258	70.015128	70.015021	70.014942
70.014899	70.014899	70.014956	70.015091	70.015330	70.015714	70.016299	70.017160	70.018409	70.020193
70.022720	70.026274	70.031241	70.038150	70.047712	70.060890	70.078976	70.103701	70.137371	70.183052
70.244807	70.327998	70.439684	70.589133	70.788478	71.053561	71.405024	71.869706	72.482430	73.288307
74.345681	75.729911	77.538223	79.895924	82.964393	86.951320	92.123871	98.825588	107.498124	118.709190
133.188575	151.874827	175.976426	207.051439	247.033015	298.338522	363.732407	445.435386	541.449931	637.199479
707.134750	743.315636	758.432277	764.275844	766.514092	767.396855	767.775691	767.969446	768.096358	768.199146
768.232210	768.379495	768.461214	768.536345	768.603511	768.661280	768.708264	768.743171	768.764849	768.772325

OXYGEN CONCENTRATION

1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
1.000000	1.000000	1.000000	.999632	.998557	.994980	.981918	.934222	.790416	.517529
.246352	.095443	.034854	.012776	.004744	.001778	.000670	.000253	.000096	.000036
.000014	.000005	.000002	.000001	.000000	.000000	.000000	.000000	.000000	.000000

OIL CONCENTRATION

-.003000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.003000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.003000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000001	.000107	.000019	-.000390	-.001072	-.001479	-.003100
.006338	.048971	.089331	.114214	.127222	.133562	.136568	.137961	.138576	.138821
.138897	.138897	.138865	.138820	.138770	.138720	.138671	.138624	.138579	.138536

JWJ

.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.109219	.332234	.592264	.782059	.891326	.947948	.975261	.988305	.994587	.997544
.998891	.999510	.999790	.999906	.999959	.999997	.999990	1.000000	1.000000	1.000000

LAST DOTM ----

2.897391318

SUM OIL ----

3.491397117

***** .049528504 2 320 20.000000000

TEMPERATURE

70.091964	70.094057	70.101115	70.113746	70.132913	70.159998	70.196901	70.246164	70.311140	70.396217
70.507099	70.651180	70.838028	71.080000	71.393046	71.797738	72.320604	72.995836	73.867499	74.992372
76.443613	78.315466	80.729339	83.841618	87.853728	93.025087	99.689774	108.277973	119.343576	133.599724
151.964697	175.621424	206.094904	245.284746	295.556345	359.634909	439.790604	534.478868	630.356076	702.360591
740.660374	756.941258	763.293492	765.727689	766.667716	767.041766	767.201610	767.279944	767.326477	767.359773
767.386945	767.410999	767.433488	767.455406	767.477464	767.500173	767.523873	767.548761	767.574908	767.602289
767.630806	767.660305	767.690592	767.721448	767.752632	767.783886	767.814941	767.845516	767.875322	767.904062
767.931433	767.957130	767.980849	768.002286	768.021147	768.037146	768.050009	768.059482	768.065330	768.067340

OXYGEN CONCENTRATION

1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
1.000000	.999999	.999639	.998612	.995251	.983141	.939090	.804444	.539747	.263665
.103662	.038085	.014009	.005221	.001966	.000744	.000283	.000108	.000041	.000016
.000006	.000002	.000001	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000

OIL CONCENTRATION

-.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	-.000043	-.000105	-.000321	-.001144	-.004137	-.011752	-.015261	.007176
.046834	.088058	.114541	.128848	.136078	.139624	.141351	.142193	.142601	.142797
.142893	.142940	.142963	.142975	.142981	.142985	.142987	.142989	.142990	.142992
.142993	.142994	.142995	.142997	.142998	.142999	.143000	.143002	.143003	.143004
.143005	.143006	.143008	.143009	.143010	.143012	.143013	.143014	.143015	.143017

JWJ

.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.312147	.568646	.763509	.878873	.940117	.971025	.985992	.993203	.996734	.998449
.999245	.999639	.999823	.999917	.999961	.999982	.999990	.999996	.999998	.999999
1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	.999999	1.000000	1.000000	1.000000

LAST DOTM ---- 2.89977724

SUM OIL ---- 7.902297676