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**MATHEMATICAL MODELING
OF THE VOLOXIDATION PROCESS**

FINAL REPORT

T.G. STANFORD

June, 1979

**Work Performed Under Contract EY-76-S-09-0944
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**UNIVERSITY OF SOUTH CAROLINA
COLLEGE OF ENGINEERING
COLUMBIA, S.C. 29209**

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COLLEGE OF ENGINEERING
COLUMBIA, SOUTH CAROLINA 29208

PREPARED FOR THE
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ABSTRACT

A mathematical model of the voloxidization process, a 'head-end' reprocessing step for the removal of volatile fission products from spent nuclear fuel, has been developed. Three types of voloxidizer operation have been considered; cocurrent operation in which the gas and solid streams flow in the same direction, countercurrent operation in which the gas and solid streams flow in opposite directions, and semi-batch operation in which the gas stream passes through the reactor while the solids remain in it and are processed batch wise. Because of the complexity of the physical and chemical processes which occur during the voloxidization process and the lack of currently available kinetic data, a global kinetic model has been adapted for this study.

Test cases for each mode of operation have been simulated using representative values of the model parameters. To process 714 kgm/day of spent nuclear fuel, using an oxidizing atmosphere containing 20 mole percent oxygen, it was found that a reactor 0.7 m in diameter and 2.49 m in length would be required for both cocurrent and countercurrent modes of operation while for semibatch operation a 0.3m^3 reactor and an 88200 sec batch processing time would be required.

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ABSTRACT

MATHEMATICAL MODELING OF THE VOLOXIDATION PROCESS

T. G. Stanford

Voloxidation is a process for the removal of volatile fission products prior to dissolution during spent nuclear fuel reprocessing. Both continuous and batch processes are being evaluated for this task. At the present time, it appears as if the rotary-kiln voloxidizer is the most attractive of the various alternatives which have been evaluated.

A series of computer programs have been written as an aid in the evaluation of processing and design parameters associated with the voloxidation process. Cocurrent, countercurrent, and semi-batch rotary-kiln operation have been simulated. The assumption made in the development of these models is that the release of tritium and other volatile fission products is directly dependent upon the amount of uranium dioxide oxidized to U_3O_8 during the voloxidation process. Kinetic expressions have been developed from available data. These are "global" kinetic expressions which take into account all of the physicochemical processes which are occurring. Material balances describing the various modes of voloxidizer operation and incorporating appropriate kinetic expressions evolve as first-order nonlinear ordinary differential equations. The computer algorithm used to solve these equations is a 4th order Runge-Kutta technique. The parameters used for illustrative cases which are presented are those which are felt to be most representative of the actual parameters which will be encountered.

CHAPTER 1.
AN OVERVIEW OF VOLOXIDATION
PROCESS DEVELOPMENT WORK

1.1 INTRODUCTION

The containment of radioactive wastes from nuclear fuel reprocessing plants has received considerable attention in the recent past. The recovery, entrapment, and disposal of volatile fission products has been the subject of an extensive design and development effort for several years.¹ The EPA (Environmental Protection Agency) and the NRC (Nuclear Regulatory Commission) have issued standards for the emission of krypton-85 and iodine-129, which are expected to take effect in 1983.² Although the EPA does not have sufficient information to propose new release standards for tritium, it does favor development of systems for its control.² The work discussed in this report is that associated with the development and design of tritium containment systems; especially the voloxidation process.

1.2 TRITIUM CONTAINMENT SYSTEMS: VOLOXIDATION

1.2.1 Evolution of the Voloxidation Process

Several alternative processes for containment of tritium emissions from nuclear fuel reprocessing facilities have been proposed.^{1,3,4,5} Of these, the voloxidation process has received most of the attention. It has been singled out by the people at Oak Ridge National Laboratory (ORNL) for extensive development work.

Voloxidation is a word derived from two others; "volatilization" and "oxidation." It is a descriptor for a process in which volatile fission products are separated from spent nuclear fuel which has been sheared into small segments. Release of the volitional fission products is facilitated by oxidation of the spent nuclear fuel. This is a "head-end" process step which would be added to a nuclear fuel reprocessing plant flowsheet between the

shearing and dissolution steps. It was felt initially that the voloxidation process would provide a means for removing krypton, xenon, iodine, and tritium from spent liquid-metal fast breeder reactor (LMFBR) fuel. Preliminary studies showed that volatilization of the tritium was almost quantitative while about 45% of the krypton and about 75% of the iodine were released during oxidation of the fuel.^{1,6,8} Hence, the primary purpose of the voloxidation process is to remove tritium from the fuel before it is dissolved for further processing. The majority of the tritium which is produced in LMFBR's will diffuse through the stainless steel cladding of the fuel elements and appear in the reactor cover gas so the removal of the remaining tritium by voloxidation is not crucial. With light water reactor (LWR) fuels, most of the tritium is retained either in the fuel matrix or in the Zircaloy cladding material. Thus, voloxidation is a necessary process step for these fuels if tritium is to be kept from contaminating the aqueous Purex streams.^{1,6,8}

1.2.2 Fundamental Development Work

Fundamental studies associated with the voloxidation process have been numerous. No attempt will be made here to review all of the pertinent work in this area. Only the results which have significance for the engineering design of the process will be presented. The reader is referred to the reports by Groenier¹ and Nicholson⁶ for more detailed reviews of these studies.

1.2.2.1 Preliminary Studies

Initial studies were conducted to evaluate the volatile fission product release potential of the voloxidation process. The following observations were made as a result of these studies:^{1,6,7}

1. Release of between 88% and 100% of the tritium contained in either LWR or LMFBR type fuel can be affected by oxidation of the fuel.

2. During oxidation, approximately 45% of the krypton and approximately 75% of the iodine were released from the fuel samples. Xenon also was not completely released from the fuel.
3. Both heating in an inert atmosphere and vacuum outgassing were found to be much less efficient in removing tritium and other volatile fission products than was voloxidation.

Thus, the voloxidation process now is felt to be the most practical method of tritium isolation even though release of other volatile fission products is less than quantitative.

1.2.2.2. Oxidation Studies

The importance of fuel oxidation was evident when results of the preliminary studies were evaluated. Consequently, a program of work was conducted to examine the factors affecting the oxidation of both LWR and LMFBR type fuels. During the course of this work it was found that:^{1,6,7}

1. Oxidation of UO_2 samples in air occurred between 350 °C and 550 °C.
2. The maximum rate of oxidation of UO_2 occurred at 480° C; the rate being 2 1/2 times slower at 450 °C and 2 times slower at 600 °C.
3. At temperatures above 500°C, sintering of the UO_2 resulted in a hard "crust" which reduced the rate of oxidation of the fuel significantly.
4. All samples of UO_2 which were completely oxidized to U_3O_8 also were fragmented.
5. Oxidation of $(\text{U,Pu})\text{O}_2$ samples occurred in a two-step process; a relatively fast oxidation to an oxygen/metal (O/M) molar ratio of approximately 2.3 followed by a much slower oxidation to an O/M ration of about 2.57. (This corresponds to a $\text{U}_3\text{O}_8\text{-PuO}_2$ mixture for the 20% Pu samples which were oxidized.)

6. First-stage oxidation of the mixed-oxide fuels occurred between 350 °C and 600 °C. No fragmentation of the samples was observed when the O/M ratio was less than 2.3.
7. Complete oxidation of the samples to an O/M ratio of about 2.57 occurred at temperatures between 480 °C and 600 °C. Samples so oxidized were found to have fragmented.
8. Samples containing 0.25 mole percent plutonium could not be oxidized to O/M ratios greater than about 2.36 even at temperatures as high as 850 °C. It was also observed that these samples did not fragment upon oxidation.

Based upon the results of these oxidation studies, the temperature at which the voloxidizer is operated will probably be between 450 °C and 500 °C. Temperatures within this range are low enough to prevent sintering of the fuel and high enough to allow the oxidation reaction to proceed at a reasonable rate.

1.2.3 Engineering Development Work

Several types of equipment have been considered as devices in which the oxidation of spent nuclear fuel could be affected. Among these equipment types are the batch tray reactor, the continuous stirred-bed reactor, and the rotary kiln.^{1,8} The engineering development work discussed here will focus upon the rotary-kiln voloxidizer; the device which, at this time, appears to offer operational advantages that the other equipment types do not. It has been determined in initial engineering development studies that:^{1,7,8}

1. The rate of oxidation of UO_2 in a rotary kiln attains a maximum at 480 °C. This reconfirms the results obtained during batch oxidation of UO_2 .
2. Agitation is essential for the complete oxidation of UO_2 . This is

especially true with clad fuel because of the smaller surface area available for oxidation.

3. An increase in the concentration of oxygen in the oxidizing atmosphere increases the rate of oxidation, but it also causes sintering of the fuel which reduces the rate of oxidation.

These engineering development studies have established the importance of agitation during fuel oxidation. They also have shown that, while some advantage is to be gained by adjusting the oxygen concentration in the oxidizing atmosphere, air is the most logical oxygen source for this process.

1.3 ENGINEERING DESIGN OF THE VOLOXIDATION PROCESS

Engineering development work has produced a great deal of design engineering information. Although it appears at this time that the rotary kiln is the best reactor type for voloxidation, many operational difficulties exist. Because of dust formation and semi-volatile fission product release, many people are encouraging closer studies of batch systems. Ratliff⁸ has reviewed the design aspects of voloxidation in detail. A discussion of both batch and continuous operation is included in his report.

It is important that many design criteria receive careful scrutiny during this period of voloxidation process evaluation. This can best be done using a mathematical model of the process. A mathematical description of the process allows one to examine the effects of various process changes; eliminating some and changing others so that optimum operation is achieved. Although not all of the necessary design data are available at this time, it is possible to make initial process simulations using the information which has been obtained during fundamental and engineering development studies. The development of a mathematical model of the voloxidation process is discussed in the remainder of this report.

CHAPTER 2

DEVELOPMENT OF THE REACTOR MODEL

2.1 INTRODUCTION

Continuous and semi-batch modes of operation are being considered for the voloxidation process. Sheared fuel segments, approximately one to two inches in length, are to be fed into a cylindrical kiln along with an oxygen rich gas stream. The kiln is equipped with internal mixing flights which enhance mixing and help dislodge the fuel from the cladding by a lift and drop action.

Design of the voloxidizer will be based on the desire to achieve complete oxidation of the fuel which has been found to be closely related to the release of volatile fission products. Thus, for continuous operation, the rotary kiln should be designed for a solids residence time that will allow complete oxidation of the fuel. The design for semi-batch operation should result in a batch processing time which will allow the fuel to be completely oxidized.

2.2 COCURRENT OPERATION

The gas feed stream to the reactor is composed of oxygen and an inert diluent such as either nitrogen or helium. The solids feed stream consists of spent nuclear fuel rods which have been chopped into pieces one to two inches in length. In cocurrent operation, the gas and solid phases pass through the reactor in the same direction. (See Figure 2.1).

2.2.1 Dispersion of Both Gas and Solid Phases

The oxygen mass balance for the reactor is

$$-G \frac{dC_{O_2}}{dz} + D_{eff} \frac{d^2 C_{O_2}}{dz^2} + r_{O_2} = 0 \quad (2.1)$$

COCURRENT

COUNTERCURRENT

SEMIBATCH

MODES OF VOLOXIDIZER OPERATION

Figure 2.1

where G is the flux of the inert gas through the reactor, C_{O_2} is the oxygen concentration based on the inert gas present, $D_{eff_{O_2}}$ is an effective dispersion coefficient for oxygen, and r_{O_2} is the volumetric rate of reaction of the oxygen based upon an empty reactor.

The uranium dioxide^{*} mass balance for the reactor is

$$-S \frac{dC_{UO_2}}{dz} + D_{eff_{UO_2}} \frac{d^2 C_{UO_2}}{dz^2} + r_{UO_2} = 0 \quad (2.2)$$

where S is the flux of inert solids (in this case the fuel cladding), C_{UO_2} is the uranium dioxide concentration based on the inert solids present, $D_{eff_{UO_2}}$ is an effective dispersion coefficient for uranium dioxide, and r_{UO_2} is the rate of reaction of the uranium dioxide based upon an empty reactor.

The boundary conditions for equations (2.1) and (2.2) are,⁹⁻¹²

$$\left[GC_{O_2} \right]_{z=0^-} = \left[GC_{O_2} - D_{eff_{O_2}} \frac{dC_{O_2}}{dz} \right]_{z=0} \quad (2.3)$$

$$\left[\frac{dC_{O_2}}{dz} \right]_{z=L} = 0 \quad (2.4)$$

$$\left[SC_{UO_2} \right]_{z=0^-} = \left[SC_{UO_2} - D_{eff_{UO_2}} \frac{dC_{UO_2}}{dz} \right]_{z=0} \quad (2.5)$$

*Little is known about the oxidation of mixed oxide fuels. The reactor models are developed for oxidation of UO_2 but apply equally to $(U,Pu)O_2$ fuels.

$$\left(\frac{dC_{UO_2}}{dz} \bigg|_{z = \ell} \right) = 0 \quad (2.6)$$

However, for this system, it is impossible to have dispersion of the reactants at the reactor entrance so equations (2.3) through (2.6) may be replaced by

$$\left(\frac{C_{O_2}}{dz} \bigg|_{z = 0} \right) = \left(C_{O_2} \bigg|_{z = 0} \right) \quad (2.7)$$

$$\left(\frac{dC_{O_2}}{dz} \bigg|_{z = 0} \right) = 0 \quad (2.8)$$

$$\left(C_{UO_2} \bigg|_{z = 0^-} \right) = \left(C_{UO_2} \bigg|_{z = 0} \right) \quad (2.9)$$

$$\left(\frac{dC_{O_2}}{dz} \bigg|_{z = 0} \right) = 0 \quad (2.10)$$

Equations (2.1), (2.2), and (2.7) through (2.10) may be written as the following equivalent first order system of differential equations.

$$\frac{d}{dz} \begin{pmatrix} c_{O_2} \\ \frac{dc_{O_2}}{dz} \\ c_{UO_2} \\ \frac{dc_{UO_2}}{dz} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & \frac{G}{D_{effO_2}} & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & \frac{S}{D_{effUO_2}} \end{pmatrix} \begin{pmatrix} c_{O_2} \\ \frac{dc_{O_2}}{dz} \\ c_{UO_2} \\ \frac{dc_{UO_2}}{dz} \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{r_{O_2}}{D_{effO_2}} \\ 0 \\ \frac{r_{UO_2}}{D_{effUO_2}} \end{pmatrix} \quad (2.11)$$

with

$$\begin{pmatrix} c_{O_2} \\ \frac{dc_{O_2}}{dz} \\ c_{UO_2} \\ \frac{dc_{UO_2}}{dz} \end{pmatrix} \bigg|_{z=0} = \begin{pmatrix} \left(c_{O_2} \big|_{z=0} \right) \\ 0 \\ \left(c_{UO_2} \big|_{z=0} \right) \\ 0 \end{pmatrix} \quad (2.12)$$

2.2.2 Negligible Gas Phase Dispersion

It is unlikely that dispersion in the gas phase will be significant.

Thus, $D_{effO_2} = 0$ and equation (2.1) becomes

$$-G \frac{dc_{O_2}}{dz} + r_{O_2} = 0 \quad (2.13)$$

with

$$c_{O_2} = \left(c_{O_2} \big|_{z=0} \right) \text{ at } z = 0 \quad (2.14)$$

at the reactor inlet.

The equations describing operation of the reactor are equations (2.13), (2.14), (2.2), (2.9), and (2.10). They may be written in the following equivalent form

$$\frac{d}{dz} \begin{pmatrix} c_{O_2} \\ c_{UO_2} \\ \frac{dc_{UO_2}}{dz} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & \frac{S}{D_{eff}^{UO_2}} \end{pmatrix} \begin{pmatrix} c_{O_2} \\ c_{UO_2} \\ \frac{dc_{UO_2}}{dz} \end{pmatrix} + \begin{pmatrix} \frac{r_{O_2}}{G} \\ 0 \\ \frac{r_{UO_2}}{D_{eff}^{UO_2}} \end{pmatrix} \quad (2.15)$$

with

$$\begin{pmatrix} c_{O_2} \\ c_{UO_2} \\ \frac{dc_{UO_2}}{dz} \end{pmatrix} \bigg|_{z=0} = \begin{pmatrix} c_{O_2} \big|_{z=0} \\ c_{UO_2} \big|_{z=0} \\ 0 \end{pmatrix} \quad (2.16)$$

2.2.3 Negligible Dispersion of Reactants

When dispersion of the solid phase is insignificant, equation (2.2) becomes

$$-S \frac{dc_{UO_2}}{dz} + r_{UO_2} = 0 \quad (2.17)$$

with

$$c_{UO_2} = \left(c_{UO_2} \big|_{z=0} \right) \text{ at } z = 0 \quad (2.18)$$

If both gas phase and solid phase dispersion may be neglected, then reactor operation is described by equations (2.13), (2.14), (2.17), and (2.18) which may be written as

$$\frac{d}{dz} \begin{pmatrix} c_{O_2} \\ c_{UO_2} \end{pmatrix} = \begin{pmatrix} \frac{r_{O_2}}{G} \\ \frac{r_{UO_2}}{S} \end{pmatrix} \quad (2.19)$$

with

$$\begin{pmatrix} c_{O_2} \\ c_{UO_2} \end{pmatrix} \bigg|_{z=0} = \begin{pmatrix} c_{O_2} \big|_{z=0} \\ c_{UO_2} \big|_{z=0} \end{pmatrix} \quad (2.20)$$

2.3 COUNTERCURRENT OPERATION

Although it would not be advantageous to operate an oxidation reactor in a countercurrent flow scheme, this case is examined for completeness. The only difference between this case and the case of cocurrent operation is that the gas phase and the solid phase move in opposite directions through the reactor. (See Figure 2.1)

2.3.1. Dispersion of Both Gas and Solid Phases

For this mode of reactor operation, the oxygen mass balance is

$$G \frac{dc_{O_2}}{dz} + D_{eff_{UO_2}} \frac{d^2 c_{O_2}}{dz^2} + r_{O_2} = 0 \quad (2.21)$$

while the uranium dioxide mass balance remains unchanged and is

$$-S \frac{dc_{UO_2}}{dz} + D_{eff_{UO_2}} \frac{d^2 c_{UO_2}}{dz^2} + r_{UO_2} = 0 \quad (2.2)$$

The boundry conditions for equation (2.21) are

$$-GC_{O_2} \Big|_{z = \ell +} = \left(-GC_{O_2} - D_{eff O_2} \frac{dC_{O_2}}{dz} \Big|_{z = \ell} \right) \quad (2.22)$$

$$\frac{dC_{O_2}}{dz} \Big|_{z = 0} = 0 \quad (2.23)$$

The boundry conditions for equation (2.2) are unchanged.

$$SC_{UO_2} \Big|_{z = 0} = \left(SC_{UO_2} - D_{eff UO_2} \frac{dC_{UO_2}}{dz} \Big|_{z = 0} \right) \quad (2.5)$$

$$\left(\frac{dC_{UO_2}}{dz} \Big|_{z = \ell} \right) = 0 \quad (2.6)$$

It is again possible to modify the boundry conditions because of the absence of reactant dispersion at the entrance to the reactor. Thus, equations (2.20), (2.5), and (2.6) become

$$\left(C_{O_2} \Big|_{z = \ell +} \right) = \left(C_{O_2} \Big|_{z = \ell} \right) = 0 \quad (2.24)$$

$$\left(\frac{dC_{O_2}}{dz} \Big|_{z = \ell} \right) = 0 \quad (2.25)$$

$$\left(c_{UO_2} \left| z = 0^- \right. \right) = \left(c_{UO_2} \left| z = 0 \right. \right) \quad (2.9)$$

$$\left(\frac{dc_{UO_2}}{dz} \left| z = 0 \right. \right) = 0 \quad (2.10)$$

One would like to formulate this problem as an initial-value problem rather than a boundary-value problem so that the problem associated with the numerical solution of boundary-value problems may be avoided.

This requires a knowledge of either $\left(c_{O_2} \left| z = 0 \right. \right)$ or $\left(c_{UO_2} \left| z = \ell \right. \right)$.

In this work $\left(c_{O_2} \left| z = 0 \right. \right)$ will be evaluated. An oxygen mass balance for the system provides the required relationship.

$$S \left(c_{UO_2} \left| z = 0 \right. \right) + G \left(c_{O_2} \left| z = \ell \right. \right) = S \left(c_{UO_2} \left| z = \ell \right. \right) +$$

$$S \left(c_{U_3O_8} \left| z = \ell \right. \right) \left(\frac{4 \text{ mole } O_2}{\text{mole } U_3O_8} \right) + G \left(c_{O_2} \left| z = 0 \right. \right)$$

The stoichiometry of the reaction is

If one defines x as the fractional conversion of uranium dioxide, then the oxygen mass balance gives

$$S \left(c_{UO_2} \Big|_{z=l} \right) + S \left(c_{UO_2} \Big|_{z=0} \right) - \left(1 - x \right)$$

$$S \left(c_{U_3O_8} \Big|_{z=l} \right) = \frac{1}{3} S \left(c_{UO_2} \Big|_{z=0} \right) \cdot x$$

and the overall oxygen mass balance becomes, upon rearrangement

$$\left(c_{O_2} \Big|_{z=0} \right) = \left(c_{O_2} \Big|_{z=l} \right) - \frac{1}{3} \frac{S}{G} \left(c_{UO_2} \Big|_{z=0} \right) \quad (2.26)$$

Equations (2.21) and (2.2) may be expressed as an equivalent system of first order differential equations

$$\frac{d}{dz} \begin{pmatrix} c_{O_2} \\ \frac{dc_{O_2}}{dz} \\ \frac{c_{UO_2}}{dz} \\ dc_{UO_2} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{G}{D_{eff_{O_2}}} & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & \frac{S}{D_{eff_{UO_2}}} \end{pmatrix} \begin{pmatrix} c_{O_2} \\ \frac{dc_{O_2}}{dz} \\ c_{UO_2} \\ \frac{dc_{UO_2}}{dz} \end{pmatrix} + \begin{pmatrix} 0 \\ -\frac{r_{O_2}}{D_{eff_{O_2}}} \\ 0 \\ -\frac{r_{UO_2}}{D_{eff_{UO_2}}} \end{pmatrix} \quad (2.27)$$

with the following boundry conditions

$$\begin{pmatrix} C_{O_2} \\ \frac{dC_{O_2}}{dz} \\ C_{UO_2} \\ \frac{dC_{UO_2}}{dz} \end{pmatrix} \bigg|_{z=0} = \begin{pmatrix} \left(C_{O_2} \big|_{z=\ell} \right) - \frac{1}{3} \frac{S}{G} \left(C_{UO_2} \big|_{z=0} \right) \\ 0 \\ \left(C_{UO_2} \big|_{z=0} \right) \\ 0 \end{pmatrix} \quad (2.28)$$

2.3.2 Negligible Gas Phase Dispersion

When there is no significant dispersion in the gas phase, the oxygen mass balance becomes

$$G \frac{dC_{O_2}}{dz} + r_{O_2} = 0 \quad (2.28)$$

with

$$C_{O_2} = C_{O_2} \big|_{z=0} \quad \text{at } z = \ell$$

As before, the relationship between $\left(C_{O_2} \big|_{z=0} \right)$ and $\left(C_{O_2} \big|_{z=\ell} \right)$ is

$$\left(C_{O_2} \big|_{z=0} \right) = \left(C_{O_2} \big|_{z=\ell} \right) - \frac{1}{3} \frac{S}{G} \left(C_{UO_2} \big|_{z=0} \right) \quad (2.26)$$

Equations (2.28), (2.26), (2.2), (2.9), and (2.10) describe the steady-state operation of the system. They may be written as the following equivalent first-order system

$$\frac{d}{dz} \begin{pmatrix} c_{O_2} \\ c_{UO_2} \\ \frac{dc_{UO_2}}{dz} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & \frac{S}{D_{effUO_2}} \end{pmatrix} \begin{pmatrix} c_{O_2} \\ c_{UO_2} \\ \frac{dc_{UO_2}}{dz} \end{pmatrix} + \begin{pmatrix} \frac{r_{O_2}}{G} \\ 0 \\ \frac{r_{UO_2}}{D_{effUO_2}} \end{pmatrix} \quad (2.29)$$

with

$$\begin{pmatrix} c_{O_2} \\ c_{UO_2} \\ \frac{dc_{UO_2}}{dz} \end{pmatrix} \bigg|_{z=0} = \begin{pmatrix} \left(c_{O_2} \big|_{z=\ell} \right) - \frac{1}{3} \frac{S}{G} \left(c_{UO_2} \big|_{z=0} \right) \\ \left(c_{UO_2} \big|_{z=0} \right) \\ 0 \end{pmatrix} \quad (2.30)$$

2.3.3 Negligible Dispersion of Reactants

Neglecting the dispersion of the solid phase, one obtains the following uranium dioxide mass balance

$$-S \frac{dc_{UO_2}}{dz} + r_{UO_2} = 0 \quad (2.17)$$

with the boundry condition

$$c_{UO_2} = \left(c_{UO_2} \Big|_{z=0} \right) \text{ at } z = 0 \quad (2.18)$$

If neither gas phase nor solid phase dispersion is felt to be significant, then operation of the system is described by the following first order non-linear differential equation

$$\frac{d}{dz} \begin{pmatrix} c_{O_2} \\ c_{UO_2} \end{pmatrix} = \begin{pmatrix} \frac{r_{O_2}}{G} \\ \frac{r_{UO_2}}{S} \end{pmatrix} \quad (2.31)$$

with the boundry condition

$$\begin{pmatrix} c_{O_2} \\ c_{UO_2} \end{pmatrix} \Big|_{z=0} = \begin{pmatrix} \left(c_{O_2} \Big|_{z=L} \right) - \frac{1}{3} \frac{S}{G} \left(c_{UO_2} \Big|_{z=0} \right) \\ \left(c_{UO_2} \Big|_{z=0} \right) \end{pmatrix} \quad (2.32)$$

2.4 SEMI-BATCH OPERATION

Solids are processed batch-wise in semi-batch operation. Spent nuclear fuel rods chopped into pieces one to two inches in length again constitute the solid material to be oxidized. The charge is placed in the kiln, heated to the reaction temperature, and then exposed to an oxidizing atmosphere consisting of oxygen and an inert gas diluent. (See Figure 2.1)

2.4.1 Dispersion of the Gas Phase and Segregation of the Solid Phase

The oxygen mass balance for the reactor is, in this case,

$$-G \frac{dc_{O_2}}{dz} + D_{eff_{O_2}} \frac{d^2c_{O_2}}{dz^2} + r_{O_2} = 0 \quad (2.1)$$

and the uranium dioxide mass balance is

$$Vr_{UO_2} = \bar{S} \frac{dc_{UO_2}}{dt} \quad (2.33)$$

where V is the volume of the reactor and $\bar{S}$ is the mass of inert solids charged to the reactor. It is to be noted that

$$r_{O_2} = r_{O_2}(z, t)$$

and

$$r_{UO_2} = r_{UO_2}(z, t)$$

The boundary conditions for equation (2.33) and equation (2.34) are

$$\left(GC_{O_2} \right|_{z=0} \right) = \left(GC_{O_2} - D_{eff_{O_2}} \frac{dC_{O_2}}{dz} \right|_{z=0} \right) \quad (2.3)$$

$$\left(\frac{dC_{O_2}}{dz} \right|_{z=l} \right) = 0 \quad (2.4)$$

$$C_{UO_2} = \left(C_{UO_2} \right|_{t=0} \right) \text{ at } t = 0 \quad (2.34)$$

As was done previously, dispersion of the gas phase at the reactor inlet is neglected. Thus, equations (2.3) and (2.4) may be replaced by

$$\left(C_{O_2} \right|_{z=0-} \right) = \left(C_{O_2} \right|_{z=0} \right) \quad (2.7)$$

$$\left(\frac{dC_{O_2}}{dz} \right|_{z=0} \right) = 0 \quad (2.8)$$

2.4.2 Segregation of the Solid Phase with Negligible Dispersion of the Gas Phase

When dispersion in the gas phase is not important, the oxygen mass balance is

$$-G \frac{dC_{O_2}}{dz} + r_{O_2} = 0 \quad (2.13)$$

which has the boundary condition

$$C_{O_2} = \left(C_{O_2} \mid z = 0 \right) \quad \text{at } z = 0 \quad (2.14)$$

This mode of reactor operation is described by equations (2.13), (2.14), (2.33), and (2.34).

2.4.3 Complete Mixing of the Solids Phase

The mathematical description of the reactor when the solids phase is completely mixed is identical to that of the previous two cases when dispersion in the gas phase is either important or can be neglected. However, when the solids phase is perfectly mixed, the uranium dioxide concentration C_{UO_2} is no longer a function of axial position in the reactor. This fact must be kept in mind when one solves the equations describing this case.

2.4.4 Perfect Mixing of Both Phases

This description of the reactor operations assumes that it is acting like a continuous stirred tank reactor (CSTR). The oxygen mass balance for CSTR operation is

$$A_c G \left(C_{O_2} \mid z = 0 \right) - A_c G \left(C_{O_2} \mid z = L \right) + V r_{O_2} = 0 \quad (2.35)$$

where A_c is the cross sectional area of the reactor. The uranium dioxide mass balance is

$$V_{r_{UO_2}} = \bar{V} \frac{dC_{UO_2}}{dt} \quad (2.33)$$

with the boundry condition

$$C_{UO_2} = \left(C_{UO_2} \Big|_{t=0} \right) \text{ at } t = 0 \quad (2.34)$$

Because the solids phase is completely mixed, the uranium dioxide concentration is a function of time but not of axial position in the reactor.

That is

$$C_{UO_2} = C_{UO_2}(t)$$

Reactor operation is thus described mathematically by equations (2.35), (2.33), and (2.34).

2.5 TEMPERATURE EFFECTS AND NON-ISOTHERMAL OPERATION

At this time, there is not sufficient data to allow one to consider the consequences of non-isothermal operation. An energy balance for any one of the several cases which have been considered would require knowledge of heat capacities for the spent reactor fuel and its oxidation products as well as a knowledge of heat of combustion data for the fuel. If this information is known, then consideration can be given to problems of start up and to accounting for a solids preheating zone in the reactor. It is important that temperature effects be examined in the voloxidizer design. Thus, it is felt

that every effort should be made to obtain the necessary data for an accurate energy analysis of the system.

2.6 DISPERSION COEFFICIENTS FOR THE SOLIDS PHASE AND THE GAS PHASE

Several of the cases considered in this development require a knowledge of the effective dispersion coefficients for the gas phase and the solids phase. Some work has been done at Oak Ridge National Laboratory (ORNL)¹⁷ in an effort to obtain solids phase dispersion coefficients.

Information about these quantities is very important for the accurate mathematical description of the voloxidizer. Thus, priority should be given to experimental determination of these dispersion coefficients.

CHAPTER 3

DEVELOPMENT OF KINETIC EXPRESSIONS FOR THE OXIDATION OF UO_2 AND $(\text{U,Pu})\text{O}_2$

3.1 INTRODUCTION

The goodness of any chemical process simulation depends on the parameters used in it. Of course, simulation of systems involving chemical reactions required a knowledge of the reaction kinetics. Voloxidation is a process which involves oxidation of either UO_2 or $(\text{U,Pu})\text{O}_2$. A large proportion of the fundamental work and the engineering development work has been focused on this aspect of the voloxidation process.⁷ It is this work which forms the basis for the kinetic expressions describing the oxidation of both UO_2 and $(\text{U,Pu})\text{O}_2$.

A lack of fundamental physicochemical data and the need for a "simple" description of the complex phenomena occurring during oxidation of UO_2 and $(\text{U,Pu})\text{O}_2$ make it desirable to develop a "global" kinetic expression for this process. The volumetric rate of oxidation of uranium dioxide is assumed to be represented as

$$r_{\text{UO}_2} = r_{\text{UO}_2}(C_{\text{UO}_2}, C_{\text{O}_2}, T, \omega) \quad (3.1)$$

where C_{UO_2} is the uranium dioxide based upon the inert solids present, C_{O_2} is the oxygen concentration based upon the inert gas present, T is the temperature at which the reaction is occurring, and ω is the rotational speed of the reactor. These four variables were chosen because they are felt to be the most important factors affecting the rate of oxidation of UO_2 and $(\text{U,Pu})\text{O}_2$.

3.2 RATE OF OXIDATION OF UO_2 AND $(\text{U,Pu})\text{O}_2$

3.2.1 Dependence of the Oxidation Rate Upon Uranium Dioxide Concentration - UO_2 Oxidation

Tennery¹³ made thermogravimetric measurements during the isothermal oxidation of uranium dioxide at several temperatures. The oxygen concentration

was kept constant at 20 mol% by passing 0.8 scfh of "breathing air" through the batch reactor. Results of these experiments are presented as weight gain versus time in Figure 3.1 and Figure 3.2. If it is assumed that the rate of oxidation of uranium dioxide has an p^{th} order dependence upon uranium dioxide concentration, then one would expect that the time dependence of the fractional conversion of UO_2 would be described by the differential equation

$$dx/dt_n = -d(1 - x) / dt_n = k(1 - x)^p \quad (3.2)$$

where

$$x = (C^{\circ}_{UO_2} - C_{UO_2}) / C^{\circ}_{UO_2} \quad (3.3)$$

is the fractional conversion of uranium dioxide and

$$t_n = t/\tau \quad (3.4)$$

is a time normalized using τ , the time required for maximum conversion of UO_2 to U_3O_8 (See Figure 3.3). Equation (3.2) has a solution of the form

$$t_n = -m(1 - x)^n + b \quad (3.5)$$

which may be differentiated to give

$$dx/dt_n = (1 - x)^{1-n}/mn = k(1 - x)^p \quad (3.6)$$

with $p = 1 - n$ and $k = 1/mn$. Equation (3.5) is used in this work to describe the t_n versus $(1 - x)$ behavior. It completely determines the fractional conversion, x , as a function of the normalized time, t_n . The procedure used to obtain the parameters in equation (3.5) is described in Appendix A. The calculations associated with the isothermal oxidation at 400 °C are also presented in this appendix. Table 3.1 presents the equations obtained

Figure 3.1

Figure 3.2

Figure 3.3

TABLE 3.1: PARAMETERS IN THE EQUATION
DESCRIBING VARIATIONS OF THE FRACTIONAL CONVERSION WITH TIME

Temperature	Break Point (BP)	Equation I	Equation II
		< BP 0 B.P. 0.0 < (1-x) < BP	> BP BP 1.0 BP < (1-x) < 1.0
400	.6	$\frac{t}{\tau} = .934 - .582(1-x)^{.363}$	$\frac{t}{\tau} = .496 - .404(1-x)^{4.245}$
450	.8	$\frac{t}{\tau} = .903 - .754(1-x)^{.528}$	$\frac{t}{\tau} = .282 - .260(1-x)^{7.518}$
475	.62	$\frac{t}{\tau} = 1.003 - .805(1-x)^{.346}$	$\frac{t}{\tau} = .394 - .344(1-x)^{3.229}$
480	.32	$\frac{t}{\tau} = -.302 + .495(1-x)^{-.164}$	$\frac{t}{\tau} = .359 - .379(1-x)^{1.541}$

at 400 °C, 450 °C, 475 °C, and 480 °C. The break-point value of $(1-x)$, where the oxidation reaction changes mechanism, is also listed in this table.

Because of the change in the reaction mechanism, there are two equations presented for each temperature. Figure 3.4 shows the temperature dependence of the parameters m , n and b in equation (3.5). Figure 3.5 shows the temperature dependence of the break-point. Since no data were available at intermediate temperatures and no clearly defined "trend" was observed, a linear relationship with temperature is assumed to hold for core parameter at all intermediate temperatures.

3.2.2 Dependence of the Oxidation Rate Upon Metal Oxide Concentration - $(U,Pu)O_2$ Oxidation

Tennery¹³ also made thermogravimetric measurements during the isothermal oxidation of $(U,Pu)O_2$ at several temperatures. The molar rates of uranium to plutonium was varied from infinity (pure uranium dioxide) to 3.0. The solid solutions were prepared by either mechanical mixing, or coprecipitation, or the "sol-gel" process. The oxidizing atmosphere was kept constant at 20 mol% by passing 0.8 scfh of "breathing air" through the batch reactor.

The increased complexity of the reaction mechanism which is associated with the formation of nonstoichiometric compounds, changes in crystal structure, and inhomogeneities, makes a kinetic description of the oxidation of mixed uranium, plutonium oxides very difficult. The information obtained from Tennery's work provides only a small glimpse at this complex process.

The only data which could be used to develop a kinetic model for the oxidation of $(U,Pu)O_2$ were obtained for coprecipitated $(U,Pu)O_2$ with a U/Pu molar ratio of 4. Analysis of the information indicates that the oxidation occurs in two stages; each of which is first order with the time dependence of the fractional conversion being described by the equation

Figure 3.4

Figure 3.5

$$(1 - x) = \exp(-kt) \quad (3.7)$$

The first stage of the oxidation occurs for fractional conversions up to 0.85. The rate constant in this case is

$$k = (143.66/\text{min}) \exp(-10K \text{ cal/gmol}/RT) \quad (3.8)$$

A similar analysis of the second stage of the oxidation proved to be inconclusive. An activation energy of 41 Kcal/gmol (cf 10 kcal/gmol for the first stage) was obtained but the error band on this value was 40%.

3.2.3 Dependence of the Oxidation Rate Upon Oxygen Concentration - UO_2 Oxidation

Watson and Clinton¹⁴ oxidized stainless steel clad uranium dioxide pieces in a 3 inch diameter by 2 inch long mini voloxidizer. The oxidation temperature was 480 °C and the rotation speed of the mini voloxidizer was 12 RPM. Mixtures of oxygen and nitrogen were passed through the reactor at a flow rate of 1.5 scfm. Oxygen concentration in the oxidizing atmosphere varied from 20 mol% to 100 mol%. Results of the experiments are presented in Figure 3.6. An analysis of this information led to the development of an equation describing the effect of oxygen concentration on the rate of oxidation of uranium dioxide. This equation is

$$f(Y_{\text{O}_2}) = 1.306 \times 10^4 Y_{\text{O}_2}^2 + 1.973 \times 10^{-3} Y_{\text{O}_2} + 9.097 \times 10^{-1} \quad (3.9)$$

Where Y_{O_2} is the molar percentage of oxygen in the gas phase. $f(Y_{\text{O}_2})$ represents a rate enhancement factor; the ratio of the rate of oxidation at an oxygen concentration Y_{O_2} to the rate of oxidation at an oxygen concentration of 20 mol%. This equation is shown graphically in Figure 3.7.

Its mathematical development is presented in Appendix B.

OXIDATION OF STAINLESS-STEEL-CLAD URANIA PELLETS IN A 3-IN-DIAM
MINIVOLOXIDIZER WITH THE PARTIAL PRESSURE OF O₂ AS A PARAMETER

Figure 3.6

Figure 3.7

3.2.4 Dependence of the Reaction Rate Upon the Rotation Speed of the Voloxidizer - UO_2 Oxidation

The effect of voloxidizer rotation speed on the rate of oxidation of stainless steel clad uranium dioxide pieces was studied in a 3 inch diameter by 2 inch long minivoloxidizer.¹⁴ The oxidizing atmosphere was kept at 20 mol% oxygen by passing oxygen through the reactor at 0.8 scfh. The rotation speed was varied from 0 to 36 RPM. Results of the experiments are presented in Figure 3.8. These data were used to determine an enhancement factor, $g(\omega)$; the ratio of the oxidation rate at a rotational speed ω to the oxidation rate at a rotational speed of 12 RPM. The equation for $g(\omega)$ is

$$g(\omega) = 9.509 \times 10^{-4} \omega^2 + 9.238 \times 10^{-3} \omega + 7.436 \times 10^{-1} \quad (3.10)$$

This equation is shown graphically in Figure 3.9. The mathematical development of it is presented in Appendix B.

3.3 KINETIC EXPRESSIONS FOR USE IN THE VOLOXIDIZER DESIGN EQUATIONS

At this point, it is possible to develop a reaction rate expression for inclusion in the voloxidizer design equations. If one includes the effect of oxygen concentration and voloxidizer rotation speed in a description of the change in the fractional conversion of uranium dioxide* with time then equations (3.6), (3.9) and (3.10) may be combined to give

$$dx/dt_n = (1 - x)/mn \cdot f(Y_{O_2})g(\omega) \quad (3.11)$$

Equation (3.11) is a dimensionless equation, but an equation describing the rate of production of uranium dioxide per unit reactor volume is required in the voloxidizer design equations. From equation (3.3) one obtains

*At this point the development will focus upon the oxidation of VO_2 . The procedure applies equally to $(U,Pu)O_2$.

Figure 3.8

EFFECT OF THE VOLOXIDIZER ROTATION
SPEED ON THE RATE OF CHANGE OF
THE FUEL FRACTIONAL CONVERSION

Figure 3.9

$$dC_{UO_2}/dt = -C_{UO_2}^0 dx/dt = -(C_{UO_2}^0/\tau) dx/dt_n \quad (3.12)$$

Equation (3.12) gives the rate of change of uranium dioxide per unit mass of zirconium; the inert solids present in the reactor. The mass of zirconium contained in a unit volume of the reactor at the inlet is

$$\tilde{\rho}_{Zr} = \omega_{Zr} \rho_{total} (A_{in}/A_c)(1 - \epsilon) \quad (3.13)$$

where ω_{Zr} is the inlet mass fraction of zirconium ρ_{total} is the total density of solids, A_{in} is the inlet reactor cross-sectional area occupied by the solids, A_c is the cross-sectional area of the reactor, and ϵ is the inlet void fraction in that part of the reactor occupied by solids. Since the reacting solids change density, one would like to specify the fraction of the reactor occupied by solids of the outlet. If $\underline{V}_{in}$ and $\underline{V}_{out}$ are the inlet and outlet solids bulk specific volumes, then

$$A_{in}/A_c = \underline{V}_{in}/\underline{V}_{out} \quad (3.14)$$

where A_{out} is the cross-sectional area occupied by solids at the reactor outlet. Using equation (3.14), equation (3.13) becomes

$$\tilde{\rho}_{Zr} = \omega_{Zr} \rho_{total} (A_{out}/A_c)(\underline{V}_{in}/\underline{V}_{out})(1 - \epsilon) \quad (3.15)$$

combining equation (3.12) with equation (3.15), one obtains

$$\tilde{\rho}_{Zr} dC_{UO_2}/dt = - \omega_{Zr} \rho_{total} (A_{out}/A_c)(\underline{V}_{in}/\underline{V}_{out})(1-\epsilon) C_{UO_2}^0 dx/dt_n \quad (3.16)$$

Which is the rate of change of uranium dioxide per unit volume of the reactor. Substituting equation (3.11) into equation (3.16) gives

$$r_{UO_2} = \frac{1}{\rho_{Zr}} \frac{dCuol}{dt} = -\omega_{Zr} \rho_{total} (A_{out}/A_c) (V_{in}/V_{out}) (1-\epsilon) C_{UO_2}^o (1-x)^{1-n/mn} * f(Y_{O_2}) g(\omega) \quad (3.17)$$

Now

$$Y_{O_2} = 100 C_{O_2} / (1 + C_{O_2}) \quad (3.18)$$

So equation (3.17) becomes

$$r_{UO_2} = \frac{\omega_{Zr} \rho_{total} (A_{out}/A_c) (V_{in}/V_o) (1-\epsilon) C_{UO_2}^o \cdot (1-x)^{1-n}}{\tau} \frac{f(100C_{O_2}/(1+C_{O_2})) g(\omega)}{mn}$$

Equation (3.19) is the equation which is needed for use in the voloxidizer design equations. A development of the constants found in this equation is presented in Appendix C.

3.4 CONCLUSIONS

The Kinetics of UO_2 and $(U,Pu)O_2$ oxidation is complex and not well understood. A better understanding of this phenomenon is required if a mathematical description of the voloxidation process is to be developed. Clearly, an extensive experimental program is needed in order to completely and adequately describe the oxidation of nuclear fuels. Such a program should be given priority as it is an important part of voloxidation process development.

From the initial studies which have been done, it appears as if tritium and other volatile fission products are released during voloxidation. However, the relationship between the release of volatile fission products and the level of oxidation of the metal oxide matrix is not known. All

design calculations depend on knowledge of this information. Thus, an experimental program to determine those factors which affect the release of volatile fission products should be considered to be an important aspect of voloxidation process development.

CHAPTER 4

DESCRIPTION OF THE VOLOXIDIZER

COMPUTER SIMULATION PROGRAMS

4.1 INTRODUCTION

Computer programs have been written to simulate three modes of voloxidizer operation; cocurrent, countercurrent, and semibatch. The programs are written in level G FORTRAN IV. In each case, solution of the appropriate differential equation provides one with a fractional conversion history, either in space (for cocurrent and countercurrent operation) or in time (for semibatch operation), of the voloxidizer.

4.2 COCURRENT OPERATION

The most likely mode of operation for the voloxidizer at this time appears to be a continuous, cocurrent one. The equation describing this operation when solids dispersion is neglected has been shown to be

$$-S \frac{dC_{UO_2}}{dz} + r_{UO_2} = 0 \quad (2.17)$$

which can be rewritten in terms of the fractional conversion of uranium dioxide as

$$dx/dz = -r_{UO_2}/SC^o_{UO_2} \quad (4.1)$$

with

$$x = 0 \text{ at } z = 0 \quad (4.2)$$

The reaction rate expression is given by the equation

$$r_{UO_2} = -\psi_{Zr} \rho_{total} (A_{out}/A_c) (V_{in}/V_{out}) (1 - \epsilon) C^o_{UO_2} (1 - x)^{1-n/\tau mn} \quad (3.19)$$

$$*f[(100 C_{O_2}/(1 + C_{O_2}))]g(\omega)$$

The stoichiometry of the reaction and the mass balance for the reactor allow one to relate the oxygen concentration to the fractional conversion of uranium dioxide. This relationship is

$$C_{O_2} = C_{O_2}^0 - 1/3(S/G)C_{UO_2}^0 x \quad (4.3)$$

Equation (4.2) may then be substituted in equation (3.19) to obtain an expression for r_{UO_2} as a function of the fractional conversion of uranium dioxide and the operating parameters of the reactor. Equations (4.1) and (4.2) along with equations (3.19) and (4.3) constitute a nonlinear first-order ordinary differential equation which describes the fractional conversion of uranium dioxide as function of axial position in the reactor. This set of equations is solved using a 4th order Runge-Kutta technique.¹⁸ The computer program used to obtain the solution to the equations is listed in Appendix D and the results of a sample program are listed in Appendix E. Execution of the program requires two DATA cards. The entries on each DATA card are described in Table 4.1.

TABLE 4.1: ENTRIES ON DATA CARDS REQUIRED FOR COMPUTER SIMULATION OF A VOLOXIDATION REACTOR

CARD 1:	X	initial axial position in the voloxidizer (meters)
	Y	fractional conversion of uranium dioxide at the initial axial position in the reactor
	H	step size used in the differential equation solving algorithm (meters)
	NP	number of incremental steps taken between values which appear in the plot of the results produced by the program
CARD 2:	E	solids void fraction
	D	diameter of the voloxidizer (meters)
	DB	voloxidizer diameter to fuel bed depth ratio at the reactor outlet
	V1	inlet specific volume of solids (cubic meters/metric ton)
*	V2	outlet specific volume of solids (cubic meters/metric ton)
*	CØ2	inlet oxygen concentration (moles O ₂ /mole diluent gas)
*	CUØ2	inlet uranium dioxide concentration (moles UO ₂ /kg Zirconium)
	RPM	voloxidizer rotation speed (RPM)
*	T	operating temperature of the voloxidizer (°C)
	TG	inlet gas temperature (°C)
*	P	operating pressure of the voloxidizer (atmospheres)
*	SS	inlet solids flow rate (kgm/day)
*	Q	inlet gas flow rate (cubic meters/minute)
	MAX	desired final fractional conversion of uranium dioxide (0.0<x<1.0)

Entries on each DATA card are in "free" FORMAT. The first entry on a card starts in column 1 and entries are separated by a blank space. The order of the entries is important so it must be followed carefully.

* Only these entries are required on Card 2 in execution of the semi-batch simulator.

4.3 COUNTERCURRENT OPERATION

The differential equation which describes the countercurrent operation of the voloxidizer when solids dispersion is neglected is, once again, equation (2.17)

$$-S \frac{dC_{UO_2}}{dz} + r_{UO_2} = 0$$

which is rewritten in terms of the fractional conversion of uranium dioxide as

$$dx/dz = r_{UO_2} / SC^o_{UO_2} \quad (4.1)$$

with

$$x = 0 \text{ at } z = 0$$

The reaction rate expression in this case is

$$r_{UO_2} = -\omega_{Zr} \rho_{total} (A_{out}/A_c) (V_{in}/V_{out}) (1 - \epsilon) C^o_{UO_2} (1 - x)^{1-n/\tau nm} f[100^\circ C_{O_2} / (1 + C_{O_2})] \cdot g(\omega) \quad (3.19)$$

As in the previous case, one must obtain a relationship between C_{O_2} and the fractional conversion of uranium dioxide in the reactor. For the counter current mode of operation, this relationship is

$$C_{O_2} = C^o_{O_2} + 1/3 S/G C^o_{UO_2} (x - x_{max}) \quad (4.4)$$

Where x_{max} is the maximum fractional conversion of uranium dioxide obtained in the reactor. Equations (4.1), (4.2), (3.19), and (4.4) constitute a nonlinear first-order ordinary differential equation which describes the fractional conversion of uranium dioxide as a function of axial position in the reactor. A 4th order Runge-Kutta technique is used to solve this set of equations.

The computer program used to obtain the solution to the equations is listed in Appendix D and the results of a sample program are listed in

Appendix E. This program has as input two DATA cards which have the entries described in Table 4.1.

Table 4.1.

4.4 SEMI-BATCH OPERATION

The differential equation describing semi-batch operation of the voloxidizer assuming perfect mixing of the solids phase is

$$Vr_{UO_2} = \bar{S} \, dC_{UO_2}/dt \quad (2.33)$$

Equation (2.33) can be written as an equation describing changes in the fractional conversion of uranium dioxide.

$$dx/dt = -Vr_{UO_2}/\bar{S}C^{\circ}_{UO_2} \quad (4.4)$$

with

$$x = 0 \text{ at } t = 0 \quad (4.5)$$

If the gas phase is also perfectly mixed, then the oxygen concentration in the reactor is given by the equation

$$A_c GC^{\circ}_{O_2} - A_c G + (V/3)r_{UO_2} = 0 \quad (2.35)$$

The reacton rate expression in this case is given by the equation

$$r_{UO_2} = -C^{\circ}_{UO_2}/\tau \cdot (1 - x)^{1-n}/mn \, f[100 \cdot C_{O_2}/(1 + C_{O_2})]g(\omega)$$

Equations (2.33), (4.5), (2.35), and (3.20) constitute a nonlinear first order ordinary differential equation which is solved using a 4th order Runge-Kutta technique. Appendix D contains a listing of the computer program and Appendix E lists results of a sample program. Two DATA cards are required for execution of the program. The entries on these cards are described in Table A.1.

4.5 MODIFICATION OF THE PROGRAMS

The computer programs used to simulate cocurrent, countercurrent, and semi-batch operation of the reactor incorporate information about the factors affecting the oxidation of uranium dioxide. If new experimental results indicate that changes in this information are warranted, then the programs are easily modified

4.5.1 Changes in the Reaction Rate Expression

A reactor rate expression of the form

$$dx/dt = (1 - x)^{1-n/mn} = k(1 - x)^p \quad (3.6)$$

is used to describe the dependence of the fractional conversion on the normalized time. The constants in this equation can easily be updated by replacement of the appropriate statements for the parameters which are found at the beginning of the program.

4.5.2 Changes in the Equation Describing the Effect of Oxygen Concentration Upon the Reaction Rate

The effect of oxygen concentration is included in the calculation of the reaction rate term. This is an ARITHMETIC FUNCTION STATEMENT for R(X,Y,M,N), which is found at the beginning of the program. This function contains in it the equation describing changes in the reaction rate with oxygen concentration which is

$$f(Y_{O_2}) = 1.306 \times 10^{-4} Y_{O_2}^2 + 1.943 \times 10^{-3} Y_{O_2} + 9.097 \times 10^{-1} \quad (3.9)$$

Either changes in the constant coefficients of this equation can be made or the equation can be replaced with one which describes more accurately the effect which the oxygen concentration has on the reaction rate.

4.5.3 Changes in the Equation Describing the Effect of Voloxidizer Rotation Speed Upon the Reaction Rate.

The variable REV in the programs is the value of $g(\omega)$ which has been determined for a particular voloxidizer rotational speed, ω . The effect of the voloxidizer rotational speed on the reaction rate was found to be

$$g(\omega) = 9.509 \times 10^{-4} \omega^2 + 9.238 \times 10^{-3} C_0 + 7.436 \times 10^{-1} \quad (3.10)$$

Replacement of this correlation with another in the programs is effected by replacing the card which defines REV with another which contains the updated information.

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NOMENCLATURE

A_c	= empty cross-sectional area of the reactor
A_{in}	= cross-sectional area of the reactor occupied by solids at the inlet
A_{out}	= cross-sectional area of the reactor occupied by solids at the outlet
CO_2	= uranium dioxide concentration based upon the inert solids present
C_{UO_2}	= uranium dioxide concentration based upon the inert solids present
$D_{eff}^{UO_2}$	= effective dispersion coefficient for uranium dioxide
G	= flux of inert gas through the reactor
K	= reaction rate constant
ℓ	= reactor length
P	= reaction order
r_{O_2}	= rate of production of oxygen per unit reactor volume
R_{UO_2}	= rate of production of uranium dioxide per unit reactor volume
S	= flux of inert solids through the reactor
$\bar{S}$	= mass of inert solids in the reactor (semi-batch operation)
V	= reactor volume
$\bar{V}_{in}$	= solids specific volume at the reactor inlet
$\bar{V}_{out}$	= solids specific volume at the reactor outlet
Y_{O_2}	= oxygen concentration in mole percent
z	= axial distance in the reactor
x	= fractional conversion of uranium dioxide in the reactor
ϵ	= solids void fraction
ω	= voloxidizer rotation speed
ω_{Zr}	= weight fraction of zirconium in the inlet solids
ρ_{total}	= solids density
$\tilde{\rho}_{Zr}$	= density of zirconium based upon unit reactor volume
τ	= time for maximum conversion of uranium dioxide to U_3O_8

APPENDIX A
DEPENDENCE OF THE RATE OF OXIDATION
UPON URANIUM DIOXIDE CONCENTRATION

A.1 INTRODUCTION

The rate of oxidation of uranium dioxide is assumed to have a p th order dependence upon uranium dioxide concentration. Thus,

$$-d(1 - x)/t_n = k(1 - x)^p \quad (3.2)$$

Where x is the fractional conversion of uranium dioxide and t_n is a time normalized using τ , the time required for maximum conversion of UO_2 to U_3O_8 . This equation has a solution of the form

$$t_n = -m(1 - x)^n + b \quad (3.5)$$

where

$$p = 1 - n$$

and

$$k = 1/mn$$

A.2 DESCRIPTION OF THE CALCULATION PROCEDURE

The parameters in equation (3.2) and equation (3.5) are obtained using the following procedure.

1. Plot $(1 - x)$ versus t_n for a given temperature T .
2. Obtain the slope of the curve, $d(1 - x)/dt_n$, as a function of t_n by graphical differentiation.
3. Plot $\log (-d(1 - x)/dt_n)$ versus $\ln(1 - x)$ and determine the slope of the best line segment which can be drawn through the data. This should be a linear graph with slope p since equation (3.2) can be written as

$$\log (-d(1-x)/dt_n) = \ln(k) + p \ln(1-x)$$

4. Determine the point of intersection between the left most two straight line segments in the plot. (Such points are defined as break-points and indicate a change in the reaction mechanism. (See Figure 3.5.))
5. Solve equation (3.2) using the initial condition

$$(1-x) = 0.0 \text{ at } t_n = 1.0$$

to obtain the constants b_1 , m_1 , and n_1 in equation (3.5). This equation describes the time dependence of the fractional conversion for

$$0.0 < (1-x) < BP_1$$

where BP_1 is the first break-point value of $(1-x)$.

6. Repeat step 5 using the initial condition

$$(1-x) = BP_1 \text{ at } t_n = t_{n1}$$

to obtain the constants in the equation

$$t_n = m_2 (1-x)^{n_2} + b_2$$

which holds for

$$BP_1 < (1-x) < BP_2$$

7. For the ℓ th line segment, repeat step 5 using the initial condition

$$(1-x) = BP_\ell \text{ at } t_n = t_{n\ell}$$

to obtain constants in the equation

$$t_n = m_\ell (1-x)^{n_\ell} + b_\ell$$

which holds for

$$BP_{(\ell-1)} < (1-x) < BP_\ell$$

8. Repeat steps 1 through 7 for each temperature.

A.3 AN EXAMPLE: EQUATION PARAMETERS FOR THE ISOTHERMAL OXIDATION OF URANIUM DIOXIDE AT 400 °C

The following example illustrates the procedure used to obtain the parameters in equation (3.5). Data for the isothermal oxidation of uranium dioxide at 400 °C are taken from Figure 3.2. The fractional conversion and normalized times are presented in Table A.1 and plotted in Figure A.1.

Slopes of the curve shown in Figure A.1 are given in Table A.2 and shown in Figure A.2 as functions of $1 - x$,

The values of $-d(1 - x)/dt_n$ can be correlated with values of $(1 - x)$ using two straight lines, the equations of which are

$$\log (-d(1 - x)/dt_n) = 0.637 \log (1 - x) + 0.675 \quad (\text{A.1})$$

for

$$0.0 < (1 - x) < 0.6$$

and

$$\log (-d(1-x)/dt_n) = -3.245 \log (1 - x) - 0.234 \quad (\text{A.3})$$

for

$$0.6 < (1 - x) < 1.0 \quad (\text{A.4})$$

Equation (A.5) is solved with the initial condition

$$1 - x = 0.0 \text{ at } t_n = 1.0 \quad (\text{A.8})$$

to give

$$t_n = -m1(1 - x)^{n1} + b2 = -0.582(1 - x)^{0.363} + 0.134 \quad (\text{A.9})$$

and equation (A.6) is solved with the initial condition

TABLE A1: FRACTIONAL CONVERSION OF UO_2
AS A FUNCTION OF TIME DURING ISOTHERMAL OXIDATION AT 400 °C

Time, t(sec)*	τ (sec) ⁺	Normalized time t/ τ	Fractional Conversion, X*	(1-x)
20.2	182.5	.111	.015	.985
30.6	182.5	.168	.035	.965
40.8	182.5	.224	.060	.940
50.9	182.5	.279	.102	.898
61.1	182.5	.335	.174	.826
71.3	182.5	.391	.269	.731
81.4	182.5	.446	.389	.611
91.8	182.5	.503	.528	.472
102.0	182.5	.559	.664	.336
112.1	182.5	.614	.775	.225
117.1	182.5	.642	.823	.177
122.2	182.5	.670	.857	.143
127.4	182.5	.698	.894	.106
137.4	182.5	.753	.940	.060
147.6	182.5	.809	.970	.030
162.4	182.5	.890	.993	.007
182.5	182.5	1.000	1.000	0.000

*Values taken from Figure 3.2

+Value taken from Figure 3.3

Figure A.1

TABLE A.2: RATE OF CHANGE OF THE FRACTIONAL
CONVERSION OF UO_2 AS A FUNCTION OF $1-x$ FOR ISOTHERMAL OXIDATION

$(1-x)^*$	$\log (1-x)$	$(\Delta(1-x)/\Delta t_n)$	$\log(-\Delta(1-x)/\Delta t_n)$
.025	-1.602	.427	-.370
.05	-1.301	.725	-.140
.10	-1.00	1.190	.076
.20	-.699	1.667	.272
.30	-.523	2.083	.319
.40	-.398	2.778	.444
.50	-.301	2.941	.468
.60	-.222	2.381	.377
.70	-.155	2.174	.337
.80	-.097	1.613	.208
.85	-.071	1.163	.066
.90	-.046	.806	-.094
.95	-.022	.490	-.310

*Values of $(1-x)$ at which $-\Delta(1-x)/\Delta t_n$ is determined by graphical differentiation of Figure A.1.

ISOTHERMAL REACTION RATE VERSUS
FRACTIONAL CONVERSION

Figure A.2

$$1 - x = 0.6 \text{ at } t_n = 0.45 \quad (\text{A.11})$$

for

$$0.6 < (1 - x) < 1.0 \quad (\text{A.4})$$

Table A.3 presents the errors incurred when equation (A.9) and equation (A.11) are used to describe the t_n versus $(1 - x)$ behavior.

TABLE A.3: ERROR RESULTING FROM THE USE OF
EQUATION (A.9) AND EQUATION (A.11) TO DESCRIBE THE t_n VERSUS $(1 - x)$
BEHAVIOR - ISOTHERMAL OXIDATION OF UO_2 AT 400 °C

$1 - x$	t_n Experimental	t_n Derived Equations	% Error
.01	.867	.825	4.84
.025	.817	.781	4.41
.05	.761	.738	3.02
.10	.700	.682	2.57
.15	.661	.642	2.87
.20	.628	.610	2.87
.25	.597	.582	2.51
.30	.572	.558	2.45
.35	.542	.536	1.11
.40	.528	.517	2.08
.45	.508	.498	1.97
.50	.483	.481	.41
.55	.469	.466	.64
.60	.450	.451	-.22
.65	.428	.431	-.70
.70	.406	.407	-.25
.75	.378	.377	.26
.80	.350	.339	3.14
.85	.317	.293	7.57
.90	.271	.238	12.18
.95	.194	.171	11.86
.975	.139	.133	4.32

APPENDIX B

DETERMINATION OF THE EFFECT OF OXYGEN CONCENTRATION AND VOLOXIDIZER ROTATION SPEED UPON THE RATE OF OXIDATION OF URANIUM DIOXIDE

B.1 OXYGEN CONCENTRATION EFFECTS

The data presented in Figure 3.6 were used to determine the effect of concentration upon the rate of oxidation of uranium dioxide. If the rate of oxidation when the oxidizing atmosphere contains 20 mol% oxygen, then it is assumed that the rate of oxidation at some other oxygen concentration is given by the relationship

$$f(Y_{O_2}) = r_{UO_2}(Y_{O_2}) / r_{UO_2}(Y_{O_2} = 20 \text{ mol}\%O_2) = t_m(Y_{O_2} = 20 \text{ mol}\%) t_m(Y_{O_2}) \quad (B.1)$$

Y_{O_2} is the mole percent oxygen in the gas phase, where r_{UO_2} is the volumetric rate of formation of uranium dioxide, and t_m is the time required for 100% conversion of the uranium dioxide, and t_m is the time form of f is assumed to be

$$f(Y_{O_2}) = aY_{O_2}^2 + bY_{O_2} + c \quad (B.2)$$

Using the "least-squares" criterion for determination of the constants a , b , and c , one must minimize the objective function I given by the equation

$$I = \sum_{i=1}^N [f_i - (aY_{O_2,i}^2 + bY_{O_2,i} + c)]^2$$

This procedure yields the following relationship for f

$$f(Y_{O_2}) = 1.306 \times 10^{-4} Y_{O_2}^2 + 1.943 \times 10^{-3} Y_{O_2} + 9.097 \times 10^{-1} \quad (B.9)$$

The values of the f_i and the $Y_{O_2,i}$ used in the calculation are given in Table

B.1.

B.2 EFFECTS OF VOLOXIDIZER ROTATION SPEED

The data presented in Figure 3.8 were used to determine the effect of the voloxidizer rotation speed upon the rate of oxidation of uranium dioxide. Using the rate of oxidation when the rotational speed is 12 RPM as a basis, the rate of oxidation at some other rotational speed can be assumed to be given by the relationship

$$g(\omega) = r_{UO_2}(\omega) / r_{UO_2}(\omega = 12 \text{ RPM}) = t_m(\omega) \quad (B.3)$$

where ω is the rotation speed of the voloxidizer in RPM, r_{UO_2} is the volumetric rate of formation of uranium dioxide, and t_m is the time required for 100% conversion of the uranium dioxide to U_3O_8 . If the functional form of g is assumed to be

$$g(\omega) = a\omega^2 + b\omega + c$$

then the "least-squares" criterion for determining the constants a , b , and c gives the objective function

$$\sum_{i=1}^N [g_i - (a\omega_i^2 + b\omega_i + c)]^2$$

Which must be minimized with respect to the constants a , b , and c . This leads to the following relationship for g

$$g(\omega) = 9.509 \times 10^{-4} \omega^2 + 9.238 \times 10^{-3} \omega + 7.436 \times 10^{-1} \quad (3.10)$$

The values of the g_i and the ω_i used in the calculation are given in Table B.2.

TABLE B.1 EFFECT OF OXYGEN CONCENTRATION UPON THE RATE OF OXIDATION OF UO_2

% Oxygen in the Gas Phase Y_{O_2i}	Time Required for 100% Conversion of UO_2 t_m (hours) ²	$f_i = t_m (Y_{O_2} = 20 \text{ mol\%}) / (Y_{O_2})$
20	2.583	1.000
40	2.155	1.199
60	1.729	1.494
80	1.358	1.902

TABLE B.2 EFFECT OF VOLOXIDIZER ROTATION SPEED UPON THE RATE OF OXIDATION OF UO_2

Rotational Speed ω (RPM)	Time Required for 100% Conversion of UO_2 t_m (hours) ²	$g_i = t_m (\omega = 12 \text{ RPM}) / t_m (\omega)$
2	3.648	1.000
6	3.464	1.053
12	2.829	1.290
36	1.226	2.976

APPENDIX C

EVALUATION OF PARAMETERS FOR THE REACTION RATE EXPRESSION

C.1 DETERMINATION OF THE VOLUME RATIO OF FUEL TO CLADDING IN A FUEL ELEMENT

The volume ratio of fuel to cladding in a fuel element is given by the equation

$$V_{\text{fuel}}/V_{\text{clad}} = \frac{\pi}{4} D_I^2 L / \frac{\pi}{4} [(D_I + 2t)^2 - D_I^2] L = D_I^2 / 4(D_I t + t^2) \quad (\text{C.1})$$

where D_I is the inside diameter of the cladding and t is the cladding thickness.
If

$$D_I = 1/2 \text{ inch} = 1.27 \times 10^{-2} \text{ m}$$

and

$$t = 0.02 \text{ inch} = 5.08 \times 10^{-4} \text{ m}$$

then

$$\begin{aligned} V_{\text{fuel}}/V_{\text{clad}} &= (1.27 \times 10^{-2} \text{ m})^2 / 4[(1.27 \times 10^{-2} \text{ m})(5.08 \times 10^{-4} \text{ m})^2] (5.08 \times 10^{-4} \text{ m}) \\ &= 6.0 \end{aligned} \quad (\text{C.2})$$

This is expected to be a typical fuel to cladding volume ratio based upon current nuclear fuel fabrication practices.

C.2 DETERMINATION OF THE SOLIDS DENSITY

The total mass of solids (fuel plus cladding) is

$$m_{\text{total}} = m_{\text{fuel}} + m_{\text{cladding}} = V_{\text{fuel}} \rho_{\text{fuel}} + V_{\text{clad}} \rho_{\text{clad}} \quad (\text{C.3})$$

Division of this equation by the total volume of the solids gives

$$\rho_{\text{total}} = m_{\text{total}}/V_{\text{total}} = (V_{\text{fuel}} \rho_{\text{fuel}} + V_{\text{clad}} \rho_{\text{clad}})/V_{\text{total}} \quad (\text{C.4})$$

Which can be simplified using equation (C.2) to yield

$$\rho_{\text{total}} = 6/7 \rho_{\text{fuel}} + 1/7 \rho_{\text{clad}}$$

The density of the fuel is 10500 kgm/m³ and the density of zirconium is 6440 kgm/m³ so equation (C.5) can be used to obtain the total solids density

$$\begin{aligned}\rho_{\text{total}} &= 6/7 (10500 \text{ kgm/m}^3) + 1/7 (6440 \text{ kgm/m}^3) \\ &= 9920 \text{ kgm/m}^3 \\ &\approx 9900 \text{ kgm/m}^3\end{aligned}$$

C.3 DETERMINATION OF THE INLET MASS FRACTION OF INERT SOLIDS

The mass fraction of inert solids (cladding) at the inlet is

$$\begin{aligned}\omega_{\text{clad}} &= m_{\text{clad}}/m_{\text{total}} = m_{\text{clad}}/(m_{\text{clad}} + m_{\text{fuel}}) \\ &= V_{\text{clad}} \rho_{\text{clad}}/(V_{\text{clad}} \rho_{\text{clad}} + V_{\text{fuel}} \rho_{\text{fuel}}) \\ &= \rho_{\text{clad}}/[\rho_{\text{clad}} + (V_{\text{fuel}}/V_{\text{clad}})\rho_{\text{fuel}}]\end{aligned}\quad (\text{C.6})$$

This equation can be simplified using equation (C.2) to give

$$\omega_{\text{clad}} = \rho_{\text{clad}}/\rho_{\text{clad}} + 6\rho_{\text{fuel}} \quad (\text{C.7})$$

For zirconium clad fuel

$$\rho_{\text{fuel}} = 10500 \text{ kgm/m}^3$$

and

$$\rho_{\text{clad}} = 6440 \text{ kgm/m}^3$$

Hence, equation (C.7) may be evaluated as

$$\begin{aligned}\omega_{\text{clad}} &= (6440 \text{ kgm/m}^3)/(6440 \text{ kgm/m}^3) + 6(10500 \text{ kgm/m}^3) \\ &= 0.09274 \text{ kgmZr/kgm total}\end{aligned}$$

C.4 DETERMINATION OF THE URANIUM DIOXIDE CONCENTRATION

The concentration of uranium dioxide is based on the inert solids (cladding material) present. Hence,

$$C^{\circ}_{UO_2} = m_{UO_2}/m_{Zr} = m_{fuel}/m_{clad} = V_{fuel} \rho_{fuel}/V_{clad} \rho_{clad} \quad (C.8)$$

Using equation (C.2), this equation becomes

$$C^{\circ}_{UO_2} = 6 \cdot \rho_{fuel}/\rho_{clad}$$

As noted in the section C.2

$$\rho_{fuel} = 10500 \text{ kgm/m}^3$$

and

$$\rho_{clad} = 6440 \text{ kgm/m}^3$$

so

$$\begin{aligned} C^{\circ}_{UO_2} &= 6 \cdot (10500 \text{ kgm/m}^3)/(6440 \text{ kgm/m}^3) = (9.783 \text{ kgm } UO_2/\text{kgm}^Zr)(\text{kgmol } 1UO_2/267\text{kgm}) \\ &= 0.0366 \text{ kgmol } 1UO_2/\text{kg } Zr \end{aligned}$$

C.5 DETERMINATION OF THE INLET SOLIDS VOID FRACTION

The void fraction for randomly packed right cylinders is calculated using a correlation presented in Unit Operations by G. G. Brown et al.¹⁶ The correlation is based upon the sphericity, ψ , defined by the equation

$$\psi = A_{sp}/A_p \frac{\text{Surface area of a sphere with } V = V_r}{\text{Surface Area of Particle}} \quad (C.9)$$

For a right cylinder with Diameter D_p and length L

$$A_p = \pi D_p^2/2$$

and

$$V_p = \pi D_p^2 L/4$$

Thus,

$$A_{sp} = \pi(6V_p/\pi)^{2/3}$$

so

$$\psi = A_{sp}/A_p = (3/2 D_p^2 L/2)^{2/3} / (D_p^2/2 + D_p L) \quad (C.10)$$

Assuming that the length of the sheared fuel segments is 2.54×10^{-2} m and that their diameter is 1.3208×10^{-2} m, equation (C.10) yields

$$\psi = [3/2(1.3208 \times 10^{-2} \text{ m})^2(2.54 \times 10^{-2} \text{ m})]^{2/3} / [1/2(1.3208 \times 10^{-2} \text{ m})^2 + (1.3208 \times 10^{-2} \text{ m})(2.54 \times 10^{-2} \text{ m})] = 0.8363$$

This value of ψ gives a porosity, ϵ of 0.42.

C.6 DETERMINATION OF THE CROSS SECTIONAL AREA OCCUPIED BY SOLIDS

Solids will not occupy the entire volume of the voloxidizer. Specification of the fuel bed depth to kiln diameter ratio at the outlet from the reactor, D/b_{out} is a task required of the design engineer. The currently accepted value of D/b_{out} is 5.6. Although values of D/b_{out} will be design specifications, the cross sectional area occupied by the solids is required in the reaction rate expression. This is easily determined once D/b has been fixed. The angle θ associated with the cord drawn a perpendicular distance b from the edge of a circle is

$$\begin{aligned} \theta &= 2\cos^{-1}(c/R) \\ &= 2\cos^{-1}[(D/2 - b)/D/2] \\ &= 2\cos^{-1}[(D - 2b)/D] \end{aligned} \quad (C.11)$$

The angle θ forms a sector of area

$$\begin{aligned}
 A_{\text{sec}} &= R^2 \theta / 2 \\
 &= D^2 \theta / 8 \\
 &= [(D - 2b)/D]/4
 \end{aligned} \tag{C.12}$$

The angle θ also has associated with it a triangle formed by the cord and two radii which have an included angle of θ . This triangle has an area

$$\begin{aligned}
 A_{\text{tri}} &= c(R^2 - c^2) \\
 &= (D/2 - b)[D^2/4 - (D/2 - b)^2]^{1/2} \\
 &= (D - 2b/2)(Db - b^2)^{1/2}
 \end{aligned}$$

Thus, the area of the segment is

$$A_{\text{seg}} = A_{\text{sec}} - A_{\text{tri}} = D^2 \cos^{-1}[(D - 2b)/2]/4 - [(D - 2b)/2](Db - b^2)^{1/2} \tag{C.13}$$

This is the cross sectional area occupied by the solids in the rotary-kiln reactor.

APPENDIX D
COMPUTER PROGRAM LISTINGS

D.1 CONCURRENT VOLOXIDIZER OPERATION

VOLOXIDATION
VOLOXIDIZER SIMULATION DESIGN

THIS PROGRAM IS A MATHEMATICAL MODEL OF THE HEAD-END TREATMENT
PROCESS (VOLOXIDATION) OF SPENT NUCLEAR WASTE .

CASE 1: CONCURRENT

THE RUNGE-KUTTA FOURTH ORDER ACCURACY IS USED TO SOLVE THE
FOLLOWING DIFFERENTIAL EQUATION :

$$DXUO2/DZ = -G(RPM) * ((1-E) * A(D,B) / AC * (VIN/VOUT)) * ((DZR/(S*TAU)) / (N*M)) * (1-XUO2) ** (1-N) * F(O2)$$

WHERE

$DXUO2/DZ$ = RATE OF CONVERSION OF UO_2 U_3O_8 WITH RESPECT TO
VOLOXIDIZER LENGTH

$G(RPM)$ = A MULTIPLICATIVE FACTOR WHICH IS A FUNCTION OF THE
VOLOXIDIZER'S ROTATION

$A(D,B)$ = CROSS SECTIONAL AREA OF VOLOXIDIZER THAT IS FILLED
WITH SOLIDS

$VIN/VOUT$ = RATIO OF INPUT TO OUTPUT OF THE SPECIFIC VOLUME
OF SOLIDS

$F(O2)$ = FUNCTION OF OXYGEN CONCENTRATION

NOTE THAT THIS PROGRAM USES A RATE EQUATION OF THE FORM

$$T/TAU = R - M * (1 - XUO2) ** N$$

AND WHERE THE RATE OF REACTION R IS DEFINED BY

$$R = D(XUO2) / D(T/TAU)$$

ALSO,

B, M, N ARE EQUATION CONSTANTS, FUNCTION OF TEMPERATURE

DEFINITION OF TERMS AND THEIR RESPECTIVE UNITS

WHERE

A = CONSTANT (UNITLESS)

AC = CROSS SECTIONAL AREA OF VOLOXIDIZER (M^2)

```

C      ADH= CROSS SECTIONAL AREA OF SOLIDS IN VOLOXIDIZER (M**2)
C      R(1,2)= ACONSTANT IN THE RATE EQUATION F(T)
C      BP= BREAK POINT, CONDITION TO CHANGE RATE EQUATION
C      CO2= INLET OXYGEN CONCENTRATION (MOLES O2/MOLES DILUENT GAS)
C      * DILUENT GAS SHOULD BE INERT, IN THIS CASE ITS NITROGEN
C      CUO2= URANIUM DIOXIDE CONCENTRATION (MOLES UO2 / KG ZIRCONIUM)
C      D= DIAMETER OF VOLOXIDIZER (M)
C      DH= DIAMETER TO FUEL DEPTH RATIO
C      DO= CONSTANT (1/4)
C      F= VOID FRACTION (UNITLESS)
C      G= FLUX OF DILUENT GAS (MOLES N2 / (SEC*M**2))
C      G1= GAS FLOW RATE (MOLES / MINUTE)
C      GAS2= MOLE FRACTION OF DILUENT GAS
C      GO= INPUT GAS FLOW RATE (M**3/MINUTE)
C      M(1,2)= A CONSTANT IN THE RATE EQUATION F(T)
C      MAX= DESIRED CONVERSION (RANGE: 0.0 TO 1.0)
C      N(1,2)= A CONSTANT IN THE RATE EQUATION F(T)
C      NP= FREQUENCY OF DATA POINT SELECTION
C      P= PRESSURE OF SYSTEM (ATM)
C      Q= RELATING UO2 TO N2 (MOLES UO2/ MOLES N2)
C      R= RADIUS OF VOLOXIDIZER (M)
C      REV= MULTIPLICATIVE FACTOR, FUNCTION OF VOLOXIDIZER ROTATION
C      RPM= ROTATIONS PER MINUTE OF VOLOXIDIZER
C      S= ZIRCONIUM FLOW RATE (KG ZR / (SEC*M**2))
C      SS= AMOUNT OF SOLIDS TO BE PROCESSED (KG / DAY)
C      T= TEMPERATURE OF VOLOXIDIZER (C)
C      TAU= RESIDENCE TIME (SECONDS)
C      TG= GAS INLET TEMPERATURE (C)
C      V1= INLET SPECIFIC VOLUME OF SOLIDS (M**3 / METRIC TON)
C      V2= OUTLET SPECIFIC VOLUME OF SOLIDS (M**3 / METRIC TON)

```

PLEASE NOTE

----- X(=) STANDS FOR VOLOXIDIZER LENGTH

----- Y(=) STANDS FOR CONVERSION

```

0001      REM N1,M1,N2,M2,XX(1000),YY(1000),CC(1000),ZZ(1000,2),MAX,M,N
0002      EQUIVALENCE (YY(1),ZZ(1,1)),(CC(1),ZZ(1,2))
0003      F(X,Y,M,N)=-REV*ADH*(1.-Y)**(1.-N)*(1.306E-4*(CO2-Q*Y)**2
0004      1+1.943E-3*(CU2-Q*Y)+9.997E-1)/(N*M)
0005      READ (5,*) X,Y,DH,D
0006      READ (5,*) F,D,DH,V1,V2,CO2,CUO2,RPM,T,TG,P,SS,GO,MAX
0007      DZS=6440.
0008      TG=16+273.15
      TAU=-41.96*1+20964.51

```

```

C
C
C
0009 AC=3.1415295*(D/2.)**2
0010 R=D/2.
0011 THETA=2.*(ARCOS((P-(D/DB))/R)*(180./3.1415295))
0012 ADH=(3.1415295*R**2*THETA/360.)-(R**2*(SIN(THETA))/2.)

C
C
C
0013 IF (T .LT. 400. .OR. T .GT. 490.) GO TO 500
0014 IF (T .GE. 400. .AND. T .LT. 450.) GO TO 50
0015 IF (T .GE. 450. .AND. T .LT. 475.) GO TO 51
0016 IF (T .GE. 475. .AND. T .LE. 490.) GO TO 52

C
C
C
CALCULATING THE PROPER CONSTANTS FOR THE RATE EQUATION

0017 50 H1=.004*T-1.0
0018 H1=-.00062*T+1.18200
0019 H1=-.00344*T+.7940
0020 H1=.0033*T-.4570
0021 H2=-.00428*T+2.20800
0022 H2=.00288*T-1.55600
0023 H2=.06546*T-21.9390
0024 GO TO 50
0025 51 HP=-.0072*T+4.04
0026 H1=.0040*T-.8970
0027 M1=-.00204*T+.1640
0028 N1=-.00728*T+3.80400
0029 H2=.0045*T-1.734
0030 H2=-.00336*T+1.2520
0031 H2=-.17156*T+84.7200
0032 GO TO 50
0033 52 HP=-.06*T+29.12
0034 H1=-.2610*T+124.978
0035 M1=.2600*T-124.305
0036 H1=-.1020*T+48.796
0037 H2=-.0070*T+3.719
0038 H2=-.0070*T+2.9810
0039 H2=-.3376*T+163.589
0040 59 PEV=9.509E-4*HP**2+9.238E-3*HP+7.436E-1
0041 GAS2=1./(CO2+1.)
0042 VBAR=0.082057*T6/P
0043 G1=G0/VBAR
0044 G=G1*GAS2/(60.*(AC-ADH))
0045 S=SS*DH/(7.*9900.*24.*3600.*ADB)
0046 A=(1.-E)*ADH*V1/(AC*V2)
0047 DD=DH/(S*TAU)
0048 Q=S*CU02/(3.*G)
0049 WRITE (6,99)
0050 99 FORMAT(1H1,///,11X,'C O U R R E N T')
0051 WRITE (6,100) H1,M1,N1,H2,H2,HP
0052 100 FORMAT (///,11X,'RATE EQUATION CONSTANTS',/12X,'-----'
1-----'/12X,'H1=',E12.5/12X,'M1=',E12.5/12X,'N1=',E12.5/12X,'H2',
22=',E12.5/12X,'H2=',E12.5/12X,'HP=',E12.5/12X,'HP=',E12.5)
0053 WRITE (6,110) AC,ADB,CO2,CU02,D,DB,F,G,G0,MAX,P
0054 110 FORMAT ('0',///,11X,'REACTOR PARAMETERS',/12X,'-----'
1'///12X,'CROSS SECTIONAL AREA',17X,'AC=',E12.5,2X,'M**2',/12X,'SOLI

```

```

2DS CROSS SECTIONAL AREA, 9X, ADB=, E12.5, 2X, M**2 / 12X, OXYGEN CON
CENTRATION, 16X, CO2=, E12.5, 2X, MOLES O2 / MOLES DILUENT GAS / 12X
4, URANIUM DIOXIDE CONCENTRATION, 6X, CUO2=, E12.5, 2X, MOLES UO2 /
5KG ZIRCONIUM / 12X, DIAMETER, 30X, D=, E12.5, 2X, M / 12X, DIAMETER T
60 FUEL DEPTH RATIO, 9X, DH=, E12.5 / 12X, VOID FRACTION, 25X, E=, E1
72.5 / 12X, FLUX OF DILUENT GAS, 19X, G=, E12.5, 2X, MOLES N2 / (SEC*M*
H**2) / 12X, INPUT GAS FLOW RATE, 18X, GQ=, E12.5, 2X, M**3 / MINUTE /
912X, DESIRED CONVERSION, 18X, MAX=, E12.5 / 12X, PRESSURE OF SYSTEM
1, 20X, P=, E12.5, 2X, AT(1))
0055 WRITE (6,120) RPM, S, SS, T, TAU, TG, V1, V2
0056 120 FORMAT (12X, 'REVOLUTION PER MINUTE', 15X, 'RPM=', E12.5, 2X, 'RPM' / 12X, '
12IPCONIUM FLOW RATE', 14X, 'S=', E12.5, 2X, 'KG ZR / (SEC*M**2)' / 12X, 'AM
COUNT OF SOLIDS TO BE PROCESSED', 5X, 'SS=', E12.5, 2X, 'KG / DAY' / 12X, '
3TEMPERATURE', 27X, 'T=', E12.5, 2X, 'C' / 12X, 'RESIDENCE TIME', 22X, 'TAU=
4.E12.5, 2X, 'SEC' / 12X, 'INLET GAS TEMPERATURE', 16X, 'TG=', E12.5, 2X, 'C'
5 / 12X, 'SOLIDS INLET SPECIFIC VOLUME', 9X, 'V1=', E12.5, 2X, 'M**3 / MT' /
612X, 'SOLIDS OUTLET SPECIFIC VOLUME', 8X, 'V2=', E12.5, 2X, 'M**3 / MT')
0057 J=1
0058 I=1
C
C
C --- INTEGRATION IS DONE USING THE RUNGE-KUTTA FOURTH ORDER ACCURACY
0059 60 CONTINUE
0060 A1=H*F(X,Y,M2,N2)
0061 A2=H*F(X+H/2.,Y+A1/2.,M2,N2)
0062 A3=H*F(X+H/2.,Y+A2/2.,M2,N2)
0063 A4=H*F(X+H,Y+A3,M2,N2)
0064 Y=Y+(A1+2.*A2+2.*A3+A4)/6.
0065 ZZAP=1.-Y
C
C
C --- CHECK FOR BREAK-POINT
0066 IF (ZZAP .LE. BP) GO TO 70
0067 X=X+H
0068 IF (MOD(I,NP) .NE. 0) GO TO 65
0069 72 XX(J)=X
0070 YY(J)=Y
C
C
C --- CALCULATE THE OUTLET OXYGEN CONCENTRATION CC(J)
0071 CC(J)=CO2-U*Y
0072 J=J+1
0073 65 CONTINUE
0074 I=I+1
0075 GO TO 60
0076 70 X=X-H
0077 L=I
0078 WRITE (6,130) J
0079 130 FORMAT (///,12X, 'DATA POINTS PRIOR TO H.P. =', I12)
C
C
C --- INTEGRATING THE SECOND PART OF THE RATE EQUATION
0080 90 CONTINUE
0081 A1=H*F(X,Y,M1,N1)
0082 A2=H*F(X+H/2.,Y+A1/2.,M1,N1)
0083 A3=H*F(X+H/2.,Y+A2/2.,M1,N1)
0084 A4=H*F(X+H,Y+A3,M1,N1)
0085 Y=Y+(A1+2.*A2+2.*A3+A4)/6.

```

```

      C
      C      CHECK FOR END-POINT (MAXIMUM CONVERSION)
      C
      0086      IF ((MAX-Y) .LE. 1E-4) GO TO 92
      0087      X=I*H
      0088      IF (MOD (L,NP) .NE. 0) GO TO 91
      0089      82 XX(J)=X
      0090      YY(J)=Y

      C
      C      CALCULATE THE OUTLET OXYGEN CONCENTRATION CC(J)
      C
      0091      CC(J)=C02-Q*Y

      C
      C      SAFETY CUTOFF NOT TO EXCEED 1000 DATA POINTS
      C
      0092      IF (J .GT. 1000) GO TO 92
      0093      J=J+1
      0094      91 CONTINUE
      0095      L=L+1
      0096      GO TO 90
      0097      92 WRITE (6,140) J
      0098      140 FORMAT (12X,'TOTAL NUMBER OF DATA POINTS=',I12)
      0099      WRITE (6,150) X
      0100      150 FORMAT (12X,'LENGTH OF VOLOXIDIZER (METERS) =',E12.5)

      C
      C      PLOT OF VOLOXIDIZER'S LENGTH (METERS) VS. CONVERSION(+) AND
      C      OUTLET OXYGEN CONCENTRATION(+)
      C
      0101      CALL PLOTS (1000,2,J-1,XX,ZZ)
      0102      GO TO 901
      0103      500 WRITE (6,900)
      0104      900 FORMAT(5X,'TEMP. RANGE FOR THIS PROGRAM IS 400-480,TRY AGAIN')
      0105      901 CONTINUE
      0106      STOP
      0107      END

```

```
0001      SUBROUTINE PLOTS(NDIM,NC,NL,X,Y)
0002      DIMENSION X(NL),Y(NDIM,NC),N(5),O(5),MT(5),P(132)
0003      DATA U,W,P,D/5*3,1H1,132*1H ,1H*,1H*,1H*,1H0,1HX/
0004      WRITE(6,40)
0005      40 FORMAT(1H1)
0006      WRITE(6,50) (D(K),K=1,NC)
0007      WRITE(6,32)
0008      50 FORMAT(/9X,5(A12))
0009      C=0.
0010      T=0.
0011      DO 10 L=1,NL
0012      DO 10 J=1,NC
0013      C=AMAX1(Y(L,J),C)
0014      10 T=AMIN1(Y(L,J),T)
0015      B=AMIN1((MI(NC)-2)/(C-1),50./AMAX1(C,-T))
0016      T=-T*B+2.5
0017      DO 20 K=1,NL
0018      DO 25 J=1,NC
0019      25 P(N(J))=P(1)
0020      P(T)=W
0021      M=T
0022      DO 65 J=1,NC
0023      N(J)=Y(K,J)*B+T
0024      P(N(J))=Q(J)
0025      65 M=MAX0(N(J),M)
0026      IF (NC.EQ.1) WRITE(6,31) X(K), (Y(K,J),J=1,NC), (P(J),J=1,M)
0027      IF (NC.EQ.2) WRITE(6,32) X(K), (Y(K,J),J=1,NC), (P(J),J=1,M)
0028      IF (NC.EQ.3) WRITE(6,33) X(K), (Y(K,J),J=1,NC), (P(J),J=1,M)
0029      IF (NC.EQ.4) WRITE(6,34) X(K), (Y(K,J),J=1,NC), (P(J),J=1,M)
0030      20 IF (NC.EQ.5) WRITE(6,35) X(K), (Y(K,J),J=1,NC), (P(J),J=1,M)
0031      31 FORMAT(G11.3,G12.4,2X,106A1)
0032      32 FORMAT(G11.3,2G12.4,2X,94A1)
0033      33 FORMAT(G11.3,3G12.4,2X,82A1)
0034      34 FORMAT(G11.3,4G12.4,2X,70A1)
0035      35 FORMAT(G11.3,5G12.4,2X,58A1)
0036      DATA MT/106,94,82,70,58/
0037      P(T)=P(1)
0038      RETURN
0039      END
```


D. COUNTERCURRENT VOLOXIDIZER OPERATION

VOLOXIDATION VOLOXIDIZER SIMULATION DESIGN

THIS PROGRAM IS A MATHEMATICAL MODEL OF THE HEAD-END TREATMENT
PROCESS (VOLOXIDATION) OF SPENT NUCLEAR WASTE.

CASE II: COUNTERCURRENT

THE RUNGE-KUTTA FOURTH ORDER ACCURACY IS USED TO SOLVE THE
FOLLOWING DIFFERENTIAL EQUATION :

$$DXUO2/DZ = -G(RPM) * ((1-E) * A(D,B) / AC * (VIN/VOUT)) * ((DZR / (S * \tau)) / (N * M)) * (1 - XUO2) ** (1 - N) * F(O2)$$

WHERE

$DXUO2/DZ$ = RATE OF CONVERSION OF UO_2 U_3O_8 WITH RESPECT TO
VOLOXIDIZER LENGTH

$G(RPM)$ = A MULTIPLICATIVE FACTOR WHICH IS A FUNCTION OF THE
VOLOXIDIZER'S ROTATION

$A(D,B)$ = CROSS SECTIONAL AREA OF VOLOXIDIZER THAT IS FILLED
WITH SOLIDS

$VIN/VOUT$ = RATIO OF INPUT TO OUTPUT OF THE SPECIFIC VOLUME
OF SOLIDS

$F(O2)$ = FUNCTION OF OXYGEN CONCENTRATION

NOTE THAT THIS PROGRAM USES A RATE EQUATION OF THE FORM

$$T/\tau = H - 1 * (1 - XUO2) ** N$$

AND WHERE THE RATE OF REACTION R IS DEFINED BY

$$R = D(XUO2) / D(T/\tau)$$

ALSO,

H, N, M ARE EQUATION CONSTANTS, FUNCTION OF TEMPERATURE

DEFINITION OF TERMS AND THEIR RESPECTIVE UNITS

WHERE

A = CONSTANT (UNITLESS)

AC = CROSS SECTIONAL AREA OF VOLOXIDIZER (M^2)

AD = CROSS SECTIONAL AREA OF SOLIDS IN VOLOXIDIZER (M^2)

```

C      P(1,2)= ACONSTANT IN THE RATE EQUATION F(T)
C      BP= BREAK POINT, CONDITION TO CHANGE RATE EQUATION
C      CO2= INLET OXYGEN CONCENTRATION (MOLES O2/MOLES DILUENT GAS)
C      * DILUENT GAS SHOULD BE INERT, IN THIS CASE ITS NITROGEN
C      CUO2= URANIUM DIOXIDE CONCENTRATION (MOLES UO2 / KG ZIRCONIUM)
C      D= DIAMETER OF VOLOXIDIZER (M)
C      DH= DIAMETER TO FUEL DEPTH RATIO
C      DD= CONSTANT (1/...)
C      E= VOID FRACTION (UNITLESS)
C      G= FLUX OF DILUENT GAS (MOLES N2 / (SEC*M**2))
C      G1= GAS FLOW RATE (MOLES / MINUTE)
C      GAS2= MOLE FRACTION OF DILUENT GAS
C      G0= INPUT GAS FLOW RATE (M**3/MINUTE)
C      M(1,2)= A CONSTANT IN THE RATE EQUATION F(T)
C      MAX= DESIRED CONVERSION (RANGE: 0.0 TO 1.0)
C      MAXY= EXTENT OF REACTION (TERM USED ONLY IN COUNTERCURRENT CASE)
C      N(1,2)= A CONSTANT IN THE RATE EQUATION F(T)
C      NP= FREQUENCY OF DATA POINT SELECTION
C      P= PRESSURE OF SYSTEM (ATM)
C      Q= RELATING UO2 TO N2 (MOLES UO2/ MOLES N2)
C      R= RADIUS OF VOLOXIDIZER (M)
C      REV= MULTIPLICATIVE FACTOR, FUNCTION OF VOLOXIDIZER ROTATION
C      RPM= ROTATIONS PER MINUTE OF VOLOXIDIZER
C      S= ZIRCONIUM FLOW RATE (KG ZR / (SEC*M**2))
C      SS= AMOUNT OF SOLIDS TO BE PROCESSED (KG / DAY)
C      T= TEMPERATURE OF VOLOXIDIZER (C)
C      TAU= RESIDENCE TIME (SECONDS)
C      TG= GAS INLET TEMPERATURE (C)
C      V1= INLET SPECIFIC VOLUME OF SOLIDS (M**3 / METRIC TON)
C      V2= OUTLET SPECIFIC VOLUME OF SOLIDS (M**3 / METRIC TON)

```

PLEASE NOTE

----- X(=) STANDS FOR VOLOXIDIZER LENGTH

----- Y(=) STANDS FOR CONVERSION

```

0001      REAL N1,M1,N2,M2,XX(1000),YY(1000),CC(1000),ZZ(1000,2),MAX,M,N
0002      EQUIVALENCE (YY(1),ZZ(1,1)),(CC(1),ZZ(1,2))
0003      F(X,Y,M,N)=-REV*A*DU*(1.-Y)**(1.-N)*(1.306E-4*(CO2+(S/G)*(CUO2*Y/
0004      13.-MAXY))**2.+1.443E-3*(CO2+(S/G)*(CUO2*Y/3.-MAXY))+.9097)/(N*M)
0005      READ (5,*) X,Y,M,NP
0006      READ (5,*) E,D,DH,V1,V2,CO2,CUO2,RPM,T,TG,P,SS,G0,MAX
0007      UZR=6440.
0008      TG=273.15
          TAU=-41.66*T+20964.51

```

C

C CALCULATING THE CROSS-SECTIONAL AREAS OF THE VOLOXIDIZER AND THE FUEL

C

```
0009 AC=3.1415295*(D/2.)**2
0010 R=R/2.
0011 THETA=2.*(ARCOS((R-(D/DH))/R)*(180./3.1415295))
0012 ADR=3.1415295*R**2*THETA/360.- (R**2*(SIN(THETA))/2.)
```

C

C

SELECTING THE RATE EQUATION (FUNCTION OF TEMPERATURE)

C

```
0013 IF (T .LT. 400. .OR. T .GT. 480.) GO TO 50
0014 IF (T .GE. 400. .AND. T .LT. 450.) GO TO 50
0015 IF (T .GE. 450. .AND. T .LT. 475.) GO TO 51
0016 IF (T .GE. 475. .AND. T .LE. 480.) GO TO 52
```

C

C

CALCULATING THE PROPER CONSTANTS FOR THE RATE EQUATION

C

```
0017 50 RP=-.004*T-1.0
0018 B1=-.00062*T+1.18200
0019 M1=-.00344*T+.7940
0020 N1=.0033*T-.9570
0021 B2=-.00428*T+2.20800
0022 M2=.00288*T-1.55600
0023 N2=.06546*T-21.9390
0024 GO TO 59
0025 51 RP=-.0072*T+4.04
0026 B1=.0040*T-.8970
0027 M1=-.00204*T+.1640
0028 N1=-.00728*T+3.80400
0029 B2=.0045*T-1.734
0030 M2=-.00336*T+1.2520
0031 N2=-.17156*T+84.7200
0032 GO TO 59
0033 52 RP=-.06*T+29.12
0034 B1=-.2610*T+124.978
0035 M1=.2600*T-124.305
0036 N1=-.1020*T+48.796
0037 P2=-.0070*T+3.719
0038 M2=-.0070*T+2.9810
0039 N2=-.3376*T+163.589
0040 59 REV=9.509F-4*RP**2+9.238F-3*RP**7.436E-1
0041 GAS2=1./(CO2+1.)
0042 VHAR=.082057*TG/P
0043 G1=GO/VHAR
0044 G=G1*GAS2/(60.*(AC-ADH))
0045 S=SS*DH/(7.*9900.*24.*3600.*ADH)
0046 A=(1.-E)*ADH*V1/(AC*V2)
0047 DU=NR/(S*TAU)
0048 Q=S*CU02/(3.*G)
0049 MAXY=CU02*MAX/3.
0050 WRITE (6,99)
0051 99 FORMAT(1H1,///,11X,'C O U N T E R P C U R R E N T')
0052 WRITE (6,100) M1,M1,N1,B2,M2,N2,RP
0053 100 FORMAT (///,11X,'RATE EQUATION CONSTANTS',/12X,1-----
1-----//12X,'B1=',E12.5/12X,'B1=',E12.5/12X,'N1=',E12.5/12X,'B
22=',E12.5/12X,'B2=',E12.5/12X,'M2=',E12.5/12X,'M2=',E12.5/12X,'RP=',E12.5)
0054 WRITE (6,110) AC,ADH,CO2,CU02,D,DH,E,G,G0,MAX,P
0055 110 FORMAT ('0',///,10X,'REACTION PARAMETERS',/12X,1-----
1'///12X,'CROSS SECTIONAL AREA',17X,'AC=',E12.5,2X,'M**2',/12X,'SOLI
```

```

2DS CROSS SECTIONAL AREA',9X,'ADR=',E12.5,2X,'M**2/12X,'OXYGEN CON
CENTRATION',16X,'CO2=',E12.5,2X,'MOLES O2 / MOLES DILUENT GAS'/12X
4,'URANIUM DIOXIDE CONCENTRATION',6X,'CUO2=',E12.5,2X,'MOLES UO2 /
5KG ZIRCONIUM'/12X,'DIAMETER',30X,'D=',E12.5,2X,'M/12X,'DIAMETER T
60 FUEL DEPTH RATIO',9X,'DH=',E12.5/12X,'VOID FRACTION',25X,'E=',E1
72.5/12X,'FLUX OF DILUENT GAS',19X,'G=',E12.5,2X,'MOLES N2 /(SEC*M*
R*2)'/12X,'INPUT GAS FLOW RATE',16X,'G0=',E12.5,2X,'M**3 / MINUTE'/
912X,'DESIRED CONVERSION',14X,'MAX=',E12.5/12X,'PRESSURE OF SYSTEM'
1.20X,'P=',E12.5,2X,'AT ')
0056 WRITE (6,120) RPM,S,SS,T,TAU,TG,V1,V2
0057 120 FORMAT(12X,'REVOLUTION PER MINUTE',15X,'RPM=',E12.5,2X,'RPM'/12X,'
1/IRCONIUM FLOW RATE',14X,'S=',E12.5,2X,'KG ZR /(SEC*M**2)'/12X,'AM
OUNT OF SOLIDS TO BE PROCESSED',5X,'SS=',E12.5,2X,'KG / DAY'/12X,'
3TEMPERATURE',27X,'T=',E12.5,2X,'C'/12X,'RESIDENCE TIME',22X,'TAU=',
4,E12.5,2X,'SEC'/12X,'INLET GAS TEMPERATURE',16X,'TG=',E12.5,2X,'C'
5/12X,'SOLIDS INLET SPECIFIC VOLUME',9X,'V1=',E12.5,2X,'M**3 / MT'/
612X,'SOLIDS OUTLET SPECIFIC VOLUME',8X,'V2=',E12.5,2X,'M**3 / MT')
0058 J=1
0059 I=1
C
C
C INTEGRATION IS DONE USING THE RUNGE-KUTTA FOURTH ORDER ACCURACY
C
0060 60 CONTINUE
0061 A1=H*F(X,Y,M2,N2)
0062 A2=H*F(X+H/2.,Y+A1/2.,2,N2)
0063 A3=H*F(X+H/2.,Y+A2/2.,2,N2)
0064 A4=H*F(X+H,Y+A3,M2,N2)
0065 Y=Y+(A1+2.*A2+2.*A3+A4)/6.
0066 ZZAP=1.-Y
C
C CHECK FOR BREAK POINT
C
0067 IF (ZZAP .IE. BP) GO TO 70
0068 X=I*H
0069 IF (MOD (I,NP) .NE. 0) GO TO 65
0070 72 XX(J)=X
0071 YY(J)=Y
C
C CALCULATE THE OUTLET OXYGEN CONCENTRATION CC(J)
C
0072 CC(J)=CO2-Q*Y
0073 J=J+1
0074 65 CONTINUE
0075 I=I+1
0076 GO TO 60
0077 70 X=X-H
0078 L=L+1
0079 WRITE (6,130) J
0080 130 FORMAT (///,12X,'DATA POINTS PRIOR TO R.P. =',I12 )
C
C INTEGRATING THE SECOND PART OF THE RATE EQUATION
C
0081 90 CONTINUE
0082 A1=H*F(X,Y,11,N1)
0083 A2=H*F(X+H/2.,Y+A1/2.,1,N1)
0084 A3=H*F(X+H/2.,Y+A2/2.,1,N1)
0085 A4=H*F(X+H,Y+A3,M1,N1)
0086 Y=Y+(A1+2.*A2+2.*A3+A4)/6.

```

C
C CHECK FOR END-POINT (MAXIMUM CONVERSION)
C

0087 IF ((MAX-Y) .LE. 1E-4) GO TO 92
0088 X=L*H
0089 IF (MOD (L,NP) .NE. 0) GO TO 91
0090 H2 XX(J)=X
0091 YY(J)=Y
0092 CC(J)=CO2-Q*Y

C
C SAFETY CUTOFF , NOT TO EXCEED 1000 DATA POINTS
C

0093 IF (J .GE. 1000) GO TO 92
0094 J=J+1
0095 91 CONTINUE
0096 L=L+1
0097 GO TO 90
0098 92 WRITE (6,140) J
0099 140 FORMAT (12X,'TOTAL NUMBER OF DATA POINTS=',I12)
0100 WRITE (6,150) X
0101 150 FORMAT (12X,'LENGTH OF VOLOXIDIZER (METERS) =',E12.5)

C
C PLOT OF VOLOXIDIZER'S LENGTH (METERS) VS. CONVERSION(+) AND
C OUTLET OXYGEN CONCENTRATION(*)
C

0102 CALL PLOTS (1000,2,J-1,XX,ZZ)
0103 GO TO 901
0104 500 WRITE (6,900)
0105 900 FORMAT(5X,'TEMP. RANGE FOR THIS PROGRAM IS 400-480,TRY AGAIN')
0106 901 CONTINUE
0107 STOP
0108 END

3 SEMI-BATCH VOLOXIDIZER OPERATION

VOLOXIDATION VOLOXIDIZER SIMULATION DESIGN

THIS PROGRAM IS A MATHEMATICAL MODEL OF THE HEAD-END TREATMENT
PROCESS (VOLOXIDATION) OF SPENT NUCLEAR WASTE .

CASE III: SEMIBATCH

THE RUNGE-KUTTA FOURTH ORDER ACCURACY IS USED TO SOLVE THE
FOLLOWING DIFFERENTIAL EQUATION ;

$$DCUO2/DT = CUO2 * (1 - XUO2) ** (1 - N) / (TAU * N * M)$$

WHERE

DCUO2/DT = RATE OF CHANGE OF UO2 CONCENTRATION WITH RESPECT
TO TIME

NOTE THAT THIS PROGRAM USES A RATE EQUATION OF THE FORM

$$1/TAU = H - M * (1 - XUO2) ** N$$

AND WHERE THE RATE OF REACTION R IS DEFINED BY
 $R = D(XUO2) / D(T/TAU)$

ALSO, R, M, N ARE EQUATION CONSTANTS, FUNCTION OF TEMPERATURE

DEFENITION OF TERMS AND THEIR RESPECTIVE UNITS
WHERE

B(1,2) = A CONSTANT IN THE RATE EQUATION F(T)
BP = BREAK POINT, CONDITION TO CHANGE RATE EQUATION
CO2 = INLET OXYGEN CONCENTRATION (MOLES O2/MOLES DILUENT GAS)
* DILUENT GAS SHOULD BE INERT, IN THIS CASE ITS NITROGEN
CUO2 = URANIUM DIOXIDE CONCENTRATION (MOLES UO2 / KG ZIRCONIUM)
G = GAS FLOW RATE (M**3 / SEC)
GAS2 = MOLE FRACTION OF DILUENT GAS
M(1,2) = A CONSTANT IN THE RATE EQUATION F(T)
MAX = DESIRED CONVERSION (RANGE: 0.0 TO 1.0)
N(1,2) = A CONSTANT IN THE RATE EQUATION F(T)
NP = FREQUENCY OF DATA POINT SELECTION
P = PRESSURE OF SYSTEM (ATM)
SS = AMOUNT OF SOLIDS TO BE PROCESSED (KG / DAY)
T = TEMPERATURE OF VOLOXIDIZER (C)
TAU = RESIDENCE TIME (SECONDS)

PLEASE NOTE
----- X(=) STANDS FOR TIME
----- Y(=) STANDS FOR CONVERSION

```
0001 REAL N1,M1,N2,M2,XX(1000),YY(1000),CC(1000),ZZ(1000,2),M,N,MAX
0002 EQUIVALENCE (YY(1),ZZ(1,1)),(CC(1),ZZ(1,2))
0003 F(X,Y,M,N)=CUO2*(1.-Y)**(1.-N)/(TAU*N*M)*(-1.)
0004 READ (5,*) X,Y,H,NP
0005 READ (5,*) V,CO2,CUO2,T,P,SS,G,MAX
```

000

TAU=-41.66*T+20964.51

C

C

SELECTING THE RATE EQUATION (FUNCTION OF TEMPERATURE)

C

0007

IF (T .LT. 400. .OR. T .GT. 480.) GO TO 500

0008

IF (T .GE. 400. .AND. T .LT. 450.) GO TO 50

0009

IF (T .GE. 450. .AND. T .LT. 475.) GO TO 51

0010

IF (T .GE. 475. .AND. T .LE. 480.) GO TO 52

C

C

CALCULATING THE PROPER CONSTANTS FOR THE RATE EQUATION

0011

50

BP=.004*T-1.0

0012

B1=-.00062*T+1.18200

0013

M1=-.00344*T+.7940

0014

N1=.0033*T-.9570

0015

H2=-.00428*T+2.20800

0016

A2=.00288*T-1.55600

0017

N2=.06546*T-21.9390

0018

GO TO 59

0019

51

HP=-.0072*T+4.04

0020

B1=.0040*T-.8970

0021

M1=-.00204*T+.1640

0022

N1=-.00728*T+3.80400

0023

H2=.0045*T-1.734

0024

M2=-.00336*T+1.2520

0025

N2=-.17156*T+84.7200

0026

GO TO 59

0027

52

HP=-.06*T+29.12

0028

B1=-.2610*T+124.978

0029

M1=.2600*T-124.305

0030

N1=-.1020*T+48.796

0031

B2=-.0070*T+3.719

0032

M2=-.0070*T+2.9810

0033

N2=-.3376*T+163.589

0034

59

CONTINUE

0035

VOR=2.*SS/9900.

0036

GAS2=1./(CO2+1.)

0037

WRITE (6,99)

0038

99

FORMAT(1H1,///,11X,'S E M I B A T C H')

0039

WRITE (6,100) B1,M1,N1,H2,M2,N2,HP

0040

100

FORMAT (////,12X,'RATE EQUATION CONSTANTS',/12X,'-----

1-----',/12X,'B1=',E12.5/12X,'M1=',E12.5/12X,'N1=',E12.5/12X,'B

22=',E12.5/12X,'M2=',E12.5/12X,'N2=',E12.5/12X,'BP=',E12.5)

0041

WRITE (6,110) CO2,COU2,G,GAS2,MAX

0042

110

FORMAT (////,11X,'REACTOR PARAMETERS',/12X,'-----

1'///12X,'OXYGEN CONCENTRATION',16X,'CO2=',E12.5,2X,'MOLES O2 / MOL

2ES DILUENT GAS',/12X,'URANIUM DIOXIDE CONCENTRATION',6X,'COU2=',E12

3.5,2X,'MOLES UO2 / KG ZIRCONIUM',/12X,'GAS FLOW RATE',25X,'G=',E12.

45,2X,'M**3 / SEC',/12X,'DILUENT GAS MOLE FRAC',14X,'GAS2=',E12.5/12

5X,'DESIRED CONVERSION',18X,'MAX=',E12.5)

0043

WRITE (6,120) P,SS,T,TAU,V

0044

120

FORMAT (12X,'PRESSURE',30X,'P=',E12.5,2X,'ATM',/12X,'AMOUNT OF SOLI

IDS TO BE PROCESSED',5X,'SS=',E12.5,2X,'KG / DAY',/12X,'TEMPERATURE',

2,27X,'T=',E12.5,2X,'C',/12X,'RESIDENCE TIME',22X,'TAU=',E12.5,2X,'S

3EC',/12X,'VOLUME OF REACTOR',21X,'V=',E12.5,2X,'M**3')

0045

J=1

0046

I=1

C

```

      C      INTEGRATION IS DONE USING THE RUNGE-KUTTA FOURTH ORDER ACCURACY
      C
0047      60 CONTINUE
0048      A1=H*F(X,Y,M2,N2)
0049      A2=H*F(X+H/2.,Y+A1/2.,M2,N2)
0050      A3=H*F(X+H/2.,Y+A2/2.,M2,N2)
0051      A4=H*F(X+H,Y+A3,M2,N2)
0052      Y=Y+(A1+2.*A2+2.*A3+A4)/6.
0053      ZZAP=1.-Y
      C
      C      CHECK FOR BREAK POINT
      C
0054      IF (ZZAP .LE. RP) GO TO 70
0055      X=X+H
0056      IF (MOD(I,NP) .NE. 0) GO TO 65
0057      72 XX(J)=X
0058      YY(J)=Y
0059      ALPH=(1.-Y)**(1.-N2)*CO2/(-3.*TAU*N2*M2)
      C
      C      CALCULATE THE OUTLET OXYGEN CONCENTRATION CC(J)
      C
0060      CC(J)=CO2-ALPH*V/G
0061      J=J+1
0062      65 CONTINUE
0063      I=I+1
0064      GO TO 60
0065      70 X=X-H
0066      L=L
0067      WRITE (6,130) J
0068      130 FORMAT (///,12X,'DATA POINTS PRIOR TO B.P. =',I12)
      C
      C      INTEGRATING THE SECOND PART OF THE RATE EQUATION
      C
0069      90 CONTINUE
0070      A1=H*F(X,Y,M1,N1)
0071      A2=H*F(X+H/2.,Y+A1/2.,M1,N1)
0072      A3=H*F(X+H/2.,Y+A2/2.,M1,N1)
0073      A4=H*F(X+H,Y+A3,M1,N1)
0074      Y=Y+(A1+2.*A2+2.*A3+A4)/6.
      C
      C      CHECK FOR END-POINT (MAXIMUM CONVERSION)
      C
0075      IF ((MAX-Y) .LE. 1E-4) GO TO 92
0076      X=X+H
0077      IF (MOD(L,NP) .NE. 0) GO TO 91
0078      82 XX(J)=X
0079      YY(J)=Y
0080      ALPH=(1.-Y)**(1.-N1)*CO2/(-3*TAU*N1*M1)
      C
      C      CALCULATE THE OUTLET OXYGEN CONCENTRATION CC(J)
      C
0081      CC(J)=CO2-ALPH*V/G
      C
      C      SAFETY CUTOFF . NOT TO EXCEED 1000 DATA POINTS
      C
0082      IF (J .GT. 1000) GO TO 92
0083      J=J+1
0084      91 CONTINUE

```



```
0085      L=L+1
0086      GO TO 90
0087      92 WRITE (6,140) J
0088      140 FORMAT (12X,'TOTAL NUMBER OF DATA POINTS=',I12)
0089      WRITE (6,150) X
0090      150 FORMAT (12X,'REQUIRED TIME FOR DESIRED CONVERSION (SEC) =',E12.5)
          C
          C      PLOT OF TIME VS. CONVERSION(+) AND OUTLET OXYGEN CONCENTRATION (*)
          C
0091      CALL PLOTS (1000,2,J-1,XX,ZZ)
0092      GO TO 901
0093      500 WRITE(6,900)
0094      900 FORMAT(5X,'TEMP. RANGE FOR THIS PROGRAM IS 400-480,TRY AGAIN')
0095      901 CONTINUE
0096      STOP
0097      END
```

```
0001      SUBROUTINE PLOTS(NDIM,NC,NL,X,Y)
0002      DIMENSION X(NL),Y(NDIM,NC),N(5),D(5),MT(5),P(132)
0003      DATA N,W,P,D/5*3,1H1,132*1H ,1H+,1H*,1H#,1H0,1HX/
0004      WRITE(6,40)
0005      40 FORMAT(1H1)
0006      WRITE(6,50) (D(K),K=1,NC)
0007      WRITE(6,32)
0008      50 FORMAT(/9X,5(A12))
0009      C=0.
0010      T=0.
0011      DO 10 L=1,NL
0012      DO 10 J=1,NC
0013      C=AMAX1(Y(L,J),C)
0014      10 T=AMIN1(Y(L,J),T)
0015      B=AMIN1((MT(NC)-2)/(C-T),50./AMAX1(C,-T))
0016      T=-T*B+2.5
0017      DO 20 K=1,NL
0018      DO 25 J=1,NC
0019      25 P(N(J))=P(1)
0020      P(T)=W
0021      M=T
0022      DO 65 J=1,NC
0023      N(J)=Y(K,J)*B+T
0024      P(N(J))=D(J)
0025      65 M=MAX0(N(J),M)
0026      IF (NC.EQ.1) WRITE(6,31) X(K), (Y(K,J),J=1,NC), (P(J),J=1,M)
0027      IF (NC.EQ.2) WRITE(6,32) X(K), (Y(K,J),J=1,NC), (P(J),J=1,M)
0028      IF (NC.EQ.3) WRITE(6,33) X(K), (Y(K,J),J=1,NC), (P(J),J=1,M)
0029      IF (NC.EQ.4) WRITE(6,34) X(K), (Y(K,J),J=1,NC), (P(J),J=1,M)
0030      20 IF (NC.EQ.5) WRITE(6,35) X(K), (Y(K,J),J=1,NC), (P(J),J=1,M)
0031      31 FORMAT(G11.3,G12.4,2X,106A1)
0032      32 FORMAT(G11.3,2G12.4,2X,94A1)
0033      33 FORMAT(G11.3,3G12.4,2X,82A1)
0034      34 FORMAT(G11.3,4G12.4,2X,70A1)
0035      35 FORMAT(G11.3,5G12.4,2X,58A1)
0036      DATA MT/106.94,82.70,58/
0037      P(T)=P(1)
0038      RETURN
0039      END
```

```
0001      SUBROUTINE PLOTS(NDIM,NC,NL,X,Y)
0002      DIMENSION X(NL),Y(NDIM,NC),N(5),D(5),MT(5),P(132)
0003      DATA N,W,P,D/5*3,1H1,132*1H ,1H*,1H*,1H*,1H0,1HX/
0004      WRITE(6,40)
0005      40 FORMAT(1H1)
0006      WRITE(6,50)(D(K),K=1,NC)
0007      WRITE(6,32)
0008      50 FORMAT(/9X,5(A12))
0009      C=0.
0010      T=0.
0011      DO 10 L=1,NL
0012      DO 10 J=1,NC
0013      C=AMAX1(Y(L,J),C)
0014      10 T=AMIN1(Y(L,J),T)
0015      R=AMIN1((MT(NC)-2)/(C-T),50./AMAX1(C,-T))
0016      T=-T*R+2.5
0017      DO 20 K=1,NL
0018      DO 25 J=1,NC
0019      25 P(N(J))=P(1)
0020      P(T)=W
0021      M=T
0022      DO 65 J=1,NC
0023      N(J)=Y(K,J)*B+T
0024      P(N(J))=D(J)
0025      65 M=MAX0(N(J),M)
0026      IF(NC.EQ.1)WRITE(6,31)X(K),(Y(K,J),J=1,NC),(P(J),J=1,M)
0027      IF(NC.EQ.2)WRITE(6,32)X(K),(Y(K,J),J=1,NC),(P(J),J=1,M)
0028      IF(NC.EQ.3)WRITE(6,33)X(K),(Y(K,J),J=1,NC),(P(J),J=1,M)
0029      IF(NC.EQ.4)WRITE(6,34)X(K),(Y(K,J),J=1,NC),(P(J),J=1,M)
0030      20 IF(NC.EQ.5)WRITE(6,35)X(K),(Y(K,J),J=1,NC),(P(J),J=1,M)
0031      31 FORMAT(G11.3,G12.4,2X,106A1)
0032      32 FORMAT(G11.3,2G12.4,2X,94A1)
0033      33 FORMAT(G11.3,3G12.4,2X,82A1)
0034      34 FORMAT(G11.3,4G12.4,2X,70A1)
0035      35 FORMAT(G11.3,5G12.4,2X,58A1)
0036      DATA MT/106,94,82,70,58/
0037      P(T)=P(1)
0038      RETURN
0039      END
```

APPENDIX E
SAMPLE PROGRAM OUTPUT

E.1 COCURRENT VOLOXIDIZER OPERATION

COCURRENT

RATE EQUATION CONSTANTS

R1=-0.30199E+00
M1= 0.49500E+00
N1=-0.16399E+00

R2= 0.35900E+00
M2=-0.37900E+00
N2= 0.15410E+01

RP= 0.32001E+00

REACTOR PARAMETERS

CROSS SECTIONAL AREA
SOLIDS CROSS SECTIONAL AREA
OXYGEN CONCENTRATION
URANIUM DIOXIDE CONCENTRATION
DIAMETER
DIAMETER TO FUEL DEPTH RATIO
VOID FRACTION
FLUX OF DILUENT GAS
INPUT GAS FLOW RATE
DESIRED CONVERSION
PRESSURE OF SYSTEM
REVOLUTION PER MINUTE
ZIRCONIUM FLOW RATE
AMOUNT OF SOLIDS TO BE PROCESSED
TEMPERATURE
RESIDENCE TIME
INLET GAS TEMPERATURE
SOLIDS INLET SPECIFIC VOLUME
SOLIDS OUTLET SPECIFIC VOLUME

AC= 0.38484E-02 M**2
ADB= 0.96733E-03 M**2
CU2= 0.25000E+00 MOLES O2 / MOLES DILUENT GAS
CUO2= 0.13700E-01 MOLES UO2 / KG ZIRCONIUM
U= 0.70000E-01 M
UB= 0.62500E+01
E= 0.74000E+00
G= 0.57284E+00 MOLES N2 / (SEC*M**2)
GQ= 0.37900E+01 M**3 / MINUTE
AX= 0.99900E+00
P= 0.10000E+01 ATM
RPM= 0.12000E+02 RPM
S= 0.79389E+00 KG ZR / (SEC*M**2)
SS= 0.71400E+03 KG / DAY
T= 0.48000E+03 C
TAU= 0.96771E+03 SEC
TG= 0.37315E+03 C
V1= 0.79000E+00 M**3 / MT
V2= 0.79000E+00 M**3 / MT

DATA POINTS PRIOR TO H.P. = 127
TOTAL NUMBER OF DATA POINTS= 499
LENGTH OF VOLOXIDIZER (METERS) = 0.24910E+01

.E-02	.4237E-02	.2500	+	*
.E-01	.8484E-02	.2499	+	*
.150E-01	.1274E-01	.2499	+	*
.280E-01	.1781E-01	.2499	+	*
.250E-01	.2128E-01	.2499	+	*
.300E-01	.2557E-01	.2498	+	*
.350E-01	.2987E-01	.2498	+	*
.400E-01	.3417E-01	.2498	+	*
.450E-01	.3849E-01	.2498	+	*
.500E-01	.4282E-01	.2497	+	*
.550E-01	.4716E-01	.2497	+	*
.600E-01	.5151E-01	.2497	+	*
.650E-01	.5587E-01	.2496	+	*
.700E-01	.6024E-01	.2496	+	*
.750E-01	.6462E-01	.2496	+	*
.800E-01	.6901E-01	.2496	+	*
.850E-01	.7342E-01	.2495	+	*
.900E-01	.7784E-01	.2495	+	*
.950E-01	.8226E-01	.2495	+	*
.100	.8670E-01	.2495	+	*
.105	.9115E-01	.2494	+	*
.110	.9561E-01	.2494	+	*
.115	.1001	.2494	+	*
.120	.1046	.2493	+	*
.125	.1091	.2493	+	*
.130	.1136	.2493	+	*
.135	.1181	.2493	+	*
.140	.1226	.2492	+	*
.145	.1272	.2492	+	*
.150	.1318	.2492	+	*
.155	.1363	.2491	+	*
.160	.1409	.2491	+	*
.165	.1455	.2491	+	*
.170	.1501	.2490	+	*
.175	.1548	.2490	+	*
.180	.1594	.2490	+	*
.185	.1641	.2490	+	*
.190	.1687	.2489	+	*
.195	.1734	.2489	+	*
.200	.1781	.2489	+	*
.205	.1828	.2488	+	*
.210	.1876	.2488	+	*
.215	.1923	.2488	+	*
.220	.1971	.2488	+	*
.225	.2018	.2487	+	*
.230	.2066	.2487	+	*
.235	.2114	.2487	+	*
.240	.2162	.2486	+	*
.245	.2211	.2486	+	*
.250	.2259	.2486	+	*
.255	.2308	.2485	+	*
.260	.2357	.2485	+	*
.265	.2406	.2485	+	*
.270	.2455	.2484	+	*
.275	.2504	.2484	+	*
.280	.2554	.2484	+	*
.285	.2604	.2484	+	*
.290	.2654	.2483	+	*
.295	.2704	.2483	+	*
.300	.2754	.2483	+	*
.305	.2804	.2482	+	*

.645	.6983	.2456
.650	.7058	.2455
.655	.7130	.2455
.660	.7200	.2454
.665	.7268	.2454
.670	.7335	.2454
.675	.7399	.2453
.680	.7462	.2453
.685	.7522	.2452
.690	.7582	.2452
.695	.7639	.2452
.700	.7695	.2451
.705	.7750	.2451
.710	.7802	.2451
.715	.7854	.2450
.720	.7904	.2450
.725	.7953	.2450
.730	.8000	.2449
.735	.8046	.2449
.740	.8091	.2449
.745	.8135	.2449
.750	.8177	.2448
.755	.8219	.2448
.760	.8259	.2448
.765	.8298	.2447
.770	.8337	.2447
.775	.8374	.2447
.780	.8410	.2447
.785	.8446	.2447
.790	.8480	.2446
.795	.8514	.2446
.800	.8546	.2446
.805	.8578	.2446
.810	.8609	.2446
.815	.8639	.2445
.820	.8669	.2445
.825	.8698	.2445
.830	.8726	.2445
.835	.8753	.2445
.840	.8780	.2444
.845	.8806	.2444
.850	.8831	.2444
.855	.8856	.2444
.860	.8890	.2444
.865	.8903	.2444
.870	.8926	.2444
.875	.8949	.2443
.880	.8971	.2443
.885	.8992	.2443
.890	.9013	.2443
.895	.9033	.2443
.900	.9053	.2443
.905	.9072	.2443
.910	.9091	.2442
.915	.9110	.2442
.920	.9128	.2442
.925	.9145	.2442
.930	.9162	.2442
.935	.9179	.2442
.940	.9196	.2442
.945	.9212	.2442
.950	.9227	.2442
.955	.9242	.2442
.960	.9257	.2441
.965	.9272	.2441

*	.2456
*	.2455
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*	.2442
*	.2442
*	.2442
*	.2442
*	.2442
*	.2442
*	.2441
*	.2441

1.31	.9788	.2438	*
1.31	.9791	.2438	*
1.31	.9795	.2438	*
	.9798	.2438	*
1.33	.9801	.2438	*
1.33	.9804	.2438	*
1.34	.9807	.2438	*
1.34	.9810	.2438	*
1.35	.9813	.2438	*
1.35	.9816	.2438	*
1.36	.9819	.2438	*
1.36	.9822	.2438	*
1.37	.9825	.2438	*
1.37	.9828	.2438	*
1.38	.9830	.2438	*
1.38	.9833	.2438	*
1.39	.9835	.2438	*
1.39	.9838	.2438	*
1.40	.9840	.2438	*
1.40	.9843	.2438	*
1.41	.9845	.2438	*
1.41	.9848	.2438	*
1.42	.9850	.2438	*
1.42	.9852	.2438	*
1.43	.9854	.2438	*
1.43	.9857	.2438	*
1.44	.9859	.2438	*
1.44	.9861	.2438	*
1.45	.9863	.2438	*
1.45	.9865	.2438	*
1.46	.9867	.2438	*
1.46	.9869	.2438	*
1.47	.9871	.2438	*
1.47	.9873	.2438	*
1.48	.9875	.2438	*
1.48	.9877	.2437	*
1.49	.9878	.2437	*
1.49	.9880	.2437	*
1.50	.9882	.2437	*
1.50	.9884	.2437	*
1.51	.9885	.2437	*
1.51	.9887	.2437	*
1.52	.9889	.2437	*
1.52	.9890	.2437	*
1.53	.9892	.2437	*
1.53	.9893	.2437	*
1.54	.9895	.2437	*
1.54	.9896	.2437	*
1.55	.9898	.2437	*
1.55	.9899	.2437	*
1.56	.9901	.2437	*
1.56	.9902	.2437	*
1.57	.9904	.2437	*
1.57	.9905	.2437	*
1.58	.9906	.2437	*
1.58	.9908	.2437	*
1.59	.9909	.2437	*
1.59	.9910	.2437	*
1.60	.9911	.2437	*
1.60	.9913	.2437	*
1.61	.9914	.2437	*
1.61	.9915	.2437	*
1.62	.9916	.2437	*
1.62	.9917	.2437	*

1.64	.9922	.2437	*	*
1.65	.9923	.2437	*	*
1.65	.9924	.2437	*	*
1.66	.9925	.2437	*	*
1.66	.9926	.2437	*	*
1.67	.9927	.2437	*	*
1.67	.9928	.2437	*	*
1.68	.9929	.2437	*	*
1.68	.9930	.2437	*	*
1.69	.9931	.2437	*	*
1.69	.9932	.2437	*	*
1.70	.9933	.2437	*	*
1.70	.9934	.2437	*	*
1.71	.9934	.2437	*	*
1.71	.9935	.2437	*	*
1.72	.9936	.2437	*	*
1.72	.9937	.2437	*	*
1.73	.9938	.2437	*	*
1.73	.9939	.2437	*	*
1.74	.9939	.2437	*	*
1.74	.9940	.2437	*	*
1.75	.9941	.2437	*	*
1.75	.9942	.2437	*	*
1.76	.9942	.2437	*	*
1.76	.9943	.2437	*	*
1.77	.9944	.2437	*	*
1.77	.9945	.2437	*	*
1.78	.9945	.2437	*	*
1.78	.9946	.2437	*	*
1.79	.9947	.2437	*	*
1.79	.9947	.2437	*	*
1.80	.9948	.2437	*	*
1.80	.9949	.2437	*	*
1.81	.9949	.2437	*	*
1.81	.9950	.2437	*	*
1.82	.9951	.2437	*	*
1.82	.9951	.2437	*	*
1.83	.9952	.2437	*	*
1.83	.9953	.2437	*	*
1.84	.9953	.2437	*	*
1.84	.9954	.2437	*	*
1.85	.9954	.2437	*	*
1.85	.9955	.2437	*	*
1.86	.9955	.2437	*	*
1.86	.9956	.2437	*	*
1.87	.9957	.2437	*	*
1.87	.9957	.2437	*	*
1.88	.9958	.2437	*	*
1.88	.9958	.2437	*	*
1.89	.9959	.2437	*	*
1.89	.9959	.2437	*	*
1.90	.9960	.2437	*	*
1.90	.9960	.2437	*	*
1.91	.9961	.2437	*	*
1.91	.9961	.2437	*	*
1.92	.9962	.2437	*	*
1.92	.9962	.2437	*	*
1.93	.9963	.2437	*	*
1.93	.9963	.2437	*	*
1.94	.9963	.2437	*	*
1.94	.9964	.2437	*	*
1.95	.9964	.2437	*	*
1.95	.9965	.2437	*	*

1.97	.9966	.2437	*
1.97	.9966	.2437	*
1.97	.9967	.2437	*
1.98	.9967	.2437	*
1.99	.9968	.2437	*
1.99	.9968	.2437	*
2.00	.9968	.2437	*
2.00	.9969	.2437	*
2.01	.9969	.2437	*
2.01	.9969	.2437	*
2.02	.9970	.2437	*
2.02	.9970	.2437	*
2.03	.9970	.2437	*
2.03	.9971	.2437	*
2.04	.9971	.2437	*
2.04	.9971	.2437	*
2.05	.9972	.2437	*
2.05	.9972	.2437	*
2.06	.9972	.2437	*
2.06	.9973	.2437	*
2.07	.9973	.2437	*
2.07	.9973	.2437	*
2.08	.9974	.2437	*
2.08	.9974	.2437	*
2.09	.9974	.2437	*
2.09	.9975	.2437	*
2.10	.9975	.2437	*
2.10	.9975	.2437	*
2.11	.9975	.2437	*
2.11	.9976	.2437	*
2.12	.9976	.2437	*
2.12	.9976	.2437	*
2.13	.9976	.2437	*
2.13	.9977	.2437	*
2.14	.9977	.2437	*
2.14	.9977	.2437	*
2.15	.9978	.2437	*
2.15	.9978	.2437	*
2.16	.9978	.2437	*
2.16	.9978	.2437	*
2.17	.9978	.2437	*
2.17	.9979	.2437	*
2.18	.9979	.2437	*
2.18	.9979	.2437	*
2.19	.9979	.2437	*
2.19	.9980	.2437	*
2.20	.9980	.2437	*
2.20	.9980	.2437	*
2.21	.9980	.2437	*
2.21	.9981	.2437	*
2.22	.9981	.2437	*
2.22	.9981	.2437	*
2.23	.9981	.2437	*
2.23	.9981	.2437	*
2.24	.9982	.2437	*
2.24	.9982	.2437	*
2.25	.9982	.2437	*
2.25	.9982	.2437	*
2.26	.9982	.2437	*
2.26	.9983	.2437	*
2.27	.9983	.2437	*
2.27	.9983	.2437	*
2.28	.9983	.2437	*
2.28	.9983	.2437	*

COUNTERCURRENT VOLOXIDIZER OPERATION

C O U N T E R C U R R E N T

RATE EQUATION CONSTANTS

R1=-0.30199E+00
M1= 0.49500E+00
N1=-0.16399E+00

R2= 0.35900E+00
M2=-0.37900E+00
N2= 0.15410E+01

RP= 0.32001E+00

REACTOR PARAMETERS

CROSS SECTIONAL AREA	AC= 0.38484E-02	M**2
SOLIDS CROSS SECTIONAL AREA	AUB= 0.96733E-03	M**2
OXYGEN CONCENTRATION	CO2= 0.25000E+00	MOLES O2 / MOLES DILUENT GAS
URANIUM DIOXIDE CONCENTRATION	CUO2= 0.13700E-01	MOLES UO2 / KG ZIRCONIUM
DIAMETER	D= 0.70000E-01	M
DIAMETER TO FUEL DEPTH RATIO	DB= 0.62500E+01	
VOID FRACTION	E= 0.74000E+00	
FLUX OF DILUENT GAS	G= 0.57284E+00	MOLES N2 / (SEC*M**2)
INPUT GAS FLOW RATE	GW= 0.37900E+01	M**3 / MINUTE
DESIRED CONVERSION	HAX= 0.99900E+00	
PRESSURE OF SYSTEM	P= 0.10000E+01	ATM
REVOLUTION PER MINUTE	RPM= 0.12000E+02	RPM
ZIRCONIUM FLOW RATE	S= 0.79389E+00	KG ZR / (SEC*M**2)
AMOUNT OF SOLIDS TO BE PROCESSED	SS= 0.71400E+03	KG / DAY
TEMPERATURE	T= 0.48000E+03	C
RESIDENCE TIME	TAU= 0.96771E+03	SEC
INLET GAS TEMPERATURE	TG= 0.37315E+03	C
SOLIDS INLET SPECIFIC VOLUME	V1= 0.79000E+00	M**3 / MT
SOLIDS OUTLET SPECIFIC VOLUME	V2= 0.79000E+00	M**3 / MT

DATA POINTS PRIOR TO R.P. = 127
TOTAL NUMBER OF DATA POINTS= 499
LENGTH OF VOLOXIDIZER (METERS) = 0.24910E+01

.500E-02	.4237F-02	.2500	+	*
.100E-01	.8484F-02	.2499	+	*
.190E-01	.1274E-01	.2499	+	*
.200E-01	.1701E-01	.2499	+	*
.290E-01	.2128F-01	.2499	+	*
.300E-01	.2557F-01	.2499	+	*
.390E-01	.2987E-01	.2498	+	*
.400E-01	.3417F-01	.2498	+	*
.490E-01	.3849E-01	.2498	+	*
.500E-01	.4282E-01	.2497	+	*
.590E-01	.4716F-01	.2497	+	*
.600E-01	.5151E-01	.2497	+	*
.690E-01	.5587E-01	.2496	+	*
.700E-01	.6024F-01	.2496	+	*
.790E-01	.6462E-01	.2496	+	*
.800E-01	.6901E-01	.2496	+	*
.890E-01	.7342F-01	.2495	+	*
.900E-01	.7784E-01	.2495	+	*
.990E-01	.8226E-01	.2495	+	*
.100	.8670F-01	.2495	+	*
.105	.9115E-01	.2494	+	*
.110	.9561E-01	.2494	+	*
.115	.1001	.2494	+	*
.120	.1046	.2493	+	*
.125	.1091	.2493	+	*
.130	.1136	.2493	+	*
.135	.1181	.2493	+	*
.140	.1226	.2492	+	*
.145	.1272	.2492	+	*
.150	.1318	.2492	+	*
.155	.1363	.2491	+	*
.160	.1409	.2491	+	*
.165	.1455	.2491	+	*
.170	.1501	.2490	+	*
.175	.1548	.2490	+	*
.180	.1594	.2490	+	*
.185	.1641	.2490	+	*
.190	.1687	.2489	+	*
.195	.1734	.2489	+	*
.200	.1781	.2489	+	*
.205	.1828	.2488	+	*
.210	.1876	.2488	+	*
.215	.1923	.2488	+	*
.220	.1971	.2488	+	*
.225	.2018	.2487	+	*
.230	.2066	.2487	+	*
.235	.2114	.2487	+	*
.240	.2162	.2486	+	*
.245	.2211	.2486	+	*
.250	.2259	.2486	+	*
.255	.2308	.2485	+	*
.260	.2357	.2485	+	*
.265	.2406	.2485	+	*
.270	.2455	.2484	+	*
.275	.2504	.2484	+	*
.280	.2554	.2484	+	*
.285	.2604	.2484	+	*
.290	.2654	.2483	+	*
.295	.2704	.2483	+	*
.300	.2754	.2483	+	*
.305	.2804	.2482	+	*

.690	.7058	.2455
.695	.7130	.2455
	.7200	.2454
	.7268	.2454
.697	.7335	.2454
.695	.7399	.2453
.680	.7462	.2453
.685	.7523	.2452
.690	.7582	.2452
.695	.7639	.2452
.700	.7695	.2451
.705	.7750	.2451
.710	.7803	.2451
.715	.7854	.2450
.720	.7904	.2450
.725	.7953	.2450
.730	.8000	.2449
.735	.8046	.2449
.740	.8091	.2449
.745	.8135	.2449
.750	.8178	.2448
.755	.8219	.2448
.760	.8259	.2448
.765	.8299	.2447
.770	.8337	.2447
.775	.8374	.2447
.780	.8410	.2447
.785	.8446	.2447
.790	.8480	.2446
.795	.8514	.2446
.800	.8546	.2446
.805	.8578	.2446
.810	.8609	.2446
.815	.8639	.2445
.820	.8669	.2445
.825	.8698	.2445
.830	.8726	.2445
.835	.8753	.2445
.840	.8780	.2444
.845	.8806	.2444
.850	.8831	.2444
.855	.8856	.2444
.860	.8880	.2444
.865	.8903	.2444
.870	.8926	.2444
.875	.8949	.2443
.880	.8971	.2443
.885	.8992	.2443
.890	.9013	.2443
.895	.9033	.2443
.900	.9053	.2443
.905	.9072	.2443
.910	.9091	.2442
.915	.9110	.2442
.920	.9128	.2442
.925	.9145	.2442
.930	.9162	.2442
.935	.9179	.2442
.940	.9196	.2442
.945	.9212	.2442
.950	.9227	.2442
.955	.9243	.2442
.960	.9257	.2441
.965	.9272	.2441

.985	.9327	.2441
.990	.9340	.2441
	.9353	.2441
1.00	.9365	.2441
1.00	.9377	.2441
1.01	.9389	.2441
1.01	.9401	.2441
1.02	.9412	.2440
1.02	.9423	.2440
1.03	.9434	.2440
1.03	.9445	.2440
1.04	.9455	.2440
1.04	.9466	.2440
1.05	.9476	.2440
1.05	.9485	.2440
1.06	.9495	.2440
1.06	.9504	.2440
1.07	.9513	.2440
1.07	.9522	.2440
1.08	.9531	.2440
1.08	.9539	.2440
1.09	.9548	.2440
1.09	.9556	.2440
1.10	.9564	.2439
1.10	.9572	.2439
1.11	.9580	.2439
1.11	.9587	.2439
1.12	.9595	.2439
1.12	.9602	.2439
1.13	.9609	.2439
1.13	.9616	.2439
1.14	.9623	.2439
1.14	.9629	.2439
1.15	.9636	.2439
1.15	.9642	.2439
1.16	.9648	.2439
1.16	.9654	.2439
1.17	.9660	.2439
1.17	.9666	.2439
1.18	.9672	.2439
1.18	.9678	.2439
1.19	.9683	.2439
1.19	.9689	.2439
1.20	.9694	.2439
1.20	.9699	.2439
1.21	.9704	.2439
1.21	.9709	.2439
1.22	.9714	.2439
1.22	.9719	.2439
1.23	.9724	.2439
1.23	.9728	.2439
1.24	.9733	.2439
1.24	.9737	.2439
1.25	.9742	.2439
1.25	.9746	.2439
1.26	.9750	.2439
1.26	.9754	.2439
1.27	.9758	.2439
1.27	.9762	.2439
1.28	.9766	.2439
1.28	.9770	.2439
1.29	.9774	.2439
1.29	.9777	.2439

1.31	.9788	.2438	*
1.31	.9791	.2438	*
1.31	.9795	.2438	*
1.31	.9798	.2438	*
1.33	.9801	.2438	*
1.33	.9804	.2438	*
1.34	.9807	.2438	*
1.34	.9810	.2438	*
1.35	.9813	.2438	*
1.35	.9816	.2438	*
1.36	.9819	.2438	*
1.36	.9822	.2438	*
1.37	.9825	.2438	*
1.37	.9828	.2438	*
1.38	.9830	.2438	*
1.38	.9833	.2438	*
1.39	.9835	.2438	*
1.39	.9838	.2438	*
1.40	.9840	.2438	*
1.40	.9843	.2438	*
1.41	.9845	.2438	*
1.41	.9848	.2438	*
1.42	.9850	.2438	*
1.42	.9852	.2438	*
1.43	.9854	.2438	*
1.43	.9857	.2438	*
1.44	.9859	.2438	*
1.44	.9861	.2438	*
1.45	.9863	.2438	*
1.45	.9865	.2438	*
1.46	.9867	.2438	*
1.46	.9869	.2438	*
1.47	.9871	.2438	*
1.47	.9873	.2438	*
1.48	.9875	.2438	*
1.48	.9877	.2437	*
1.49	.9878	.2437	*
1.49	.9880	.2437	*
1.50	.9882	.2437	*
1.50	.9884	.2437	*
1.51	.9885	.2437	*
1.51	.9887	.2437	*
1.52	.9889	.2437	*
1.52	.9890	.2437	*
1.53	.9892	.2437	*
1.53	.9893	.2437	*
1.54	.9895	.2437	*
1.54	.9896	.2437	*
1.55	.9898	.2437	*
1.55	.9899	.2437	*
1.56	.9901	.2437	*
1.56	.9902	.2437	*
1.57	.9904	.2437	*
1.57	.9905	.2437	*
1.58	.9906	.2437	*
1.58	.9908	.2437	*
1.59	.9909	.2437	*
1.59	.9910	.2437	*
1.60	.9911	.2437	*
1.60	.9913	.2437	*
1.61	.9914	.2437	*
1.61	.9915	.2437	*
1.62	.9916	.2437	*
1.62	.9917	.2437	*

1.64	.9921	.2437	*
1.64	.9922	.2437	*
1.64	.9923	.2437	*
1.64	.9924	.2437	*
1.66	.9925	.2437	*
1.66	.9926	.2437	*
1.67	.9927	.2437	*
1.67	.9928	.2437	*
1.68	.9929	.2437	*
1.68	.9930	.2437	*
1.69	.9931	.2437	*
1.69	.9932	.2437	*
1.70	.9933	.2437	*
1.70	.9934	.2437	*
1.71	.9934	.2437	*
1.71	.9935	.2437	*
1.72	.9936	.2437	*
1.72	.9937	.2437	*
1.73	.9938	.2437	*
1.73	.9939	.2437	*
1.74	.9939	.2437	*
1.74	.9940	.2437	*
1.75	.9941	.2437	*
1.75	.9942	.2437	*
1.76	.9942	.2437	*
1.76	.9943	.2437	*
1.77	.9944	.2437	*
1.77	.9945	.2437	*
1.78	.9945	.2437	*
1.78	.9946	.2437	*
1.79	.9947	.2437	*
1.79	.9947	.2437	*
1.80	.9948	.2437	*
1.80	.9949	.2437	*
1.81	.9949	.2437	*
1.81	.9950	.2437	*
1.82	.9951	.2437	*
1.82	.9951	.2437	*
1.83	.9952	.2437	*
1.83	.9953	.2437	*
1.84	.9953	.2437	*
1.84	.9954	.2437	*
1.85	.9954	.2437	*
1.85	.9955	.2437	*
1.86	.9955	.2437	*
1.86	.9956	.2437	*
1.87	.9957	.2437	*
1.87	.9957	.2437	*
1.88	.9958	.2437	*
1.88	.9958	.2437	*
1.89	.9959	.2437	*
1.89	.9959	.2437	*
1.90	.9960	.2437	*
1.90	.9960	.2437	*
1.91	.9961	.2437	*
1.91	.9961	.2437	*
1.92	.9962	.2437	*
1.92	.9962	.2437	*
1.93	.9963	.2437	*
1.93	.9963	.2437	*
1.94	.9963	.2437	*
1.94	.9964	.2437	*
1.95	.9964	.2437	*
1.95	.9965	.2437	*

1.97	.9966	.2437
1.97	.9966	.2437
1.97	.9967	.2437
1.97	.9967	.2437
1.99	.9968	.2437
1.99	.9968	.2437
2.00	.9968	.2437
2.00	.9969	.2437
2.01	.9969	.2437
2.01	.9969	.2437
2.02	.9970	.2437
2.02	.9970	.2437
2.03	.9970	.2437
2.03	.9971	.2437
2.04	.9971	.2437
2.04	.9971	.2437
2.05	.9972	.2437
2.05	.9972	.2437
2.06	.9972	.2437
2.06	.9973	.2437
2.07	.9973	.2437
2.07	.9973	.2437
2.08	.9974	.2437
2.08	.9974	.2437
2.09	.9974	.2437
2.09	.9975	.2437
2.10	.9975	.2437
2.10	.9975	.2437
2.11	.9975	.2437
2.11	.9976	.2437
2.12	.9976	.2437
2.12	.9976	.2437
2.13	.9976	.2437
2.13	.9977	.2437
2.14	.9977	.2437
2.14	.9977	.2437
2.15	.9978	.2437
2.15	.9978	.2437
2.16	.9978	.2437
2.16	.9978	.2437
2.17	.9979	.2437
2.17	.9979	.2437
2.18	.9979	.2437
2.18	.9979	.2437
2.19	.9979	.2437
2.19	.9980	.2437
2.20	.9980	.2437
2.20	.9980	.2437
2.21	.9980	.2437
2.21	.9981	.2437
2.22	.9981	.2437
2.22	.9981	.2437
2.23	.9981	.2437
2.23	.9981	.2437
2.24	.9982	.2437
2.24	.9982	.2437
2.25	.9982	.2437
2.25	.9982	.2437
2.26	.9982	.2437
2.26	.9983	.2437
2.27	.9983	.2437
2.27	.9983	.2437
2.28	.9983	.2437
2.28	.9983	.2437

2.29	.9983	.2437
2.29	.9984	.2437
2.30	.9984	.2437
2.30	.9984	.2437
2.31	.9984	.2437
2.31	.9984	.2437
2.32	.9984	.2437
2.32	.9985	.2437
2.33	.9985	.2437
2.33	.9985	.2437
2.34	.9985	.2437
2.34	.9985	.2437
2.35	.9985	.2437
2.35	.9986	.2437
2.36	.9986	.2437
2.36	.9986	.2437
2.37	.9986	.2437
2.37	.9986	.2437
2.38	.9986	.2437
2.38	.9986	.2437
2.39	.9987	.2437
2.39	.9987	.2437
2.40	.9987	.2437
2.40	.9987	.2437
2.41	.9987	.2437
2.41	.9987	.2437
2.42	.9987	.2437
2.42	.9987	.2437
2.43	.9988	.2437
2.43	.9988	.2437
2.44	.9988	.2437
2.44	.9988	.2437
2.45	.9988	.2437
2.45	.9988	.2437
2.46	.9988	.2437
2.46	.9988	.2437
2.47	.9989	.2437
2.47	.9989	.2437
2.48	.9989	.2437
2.48	.9989	.2437
2.49	.9989	.2437

SEMI-BATCH VOLOXIDIZER OPERATION

SEMI-BATCH

RATE EQUATION CONSTANTS

R1=-0.30199E+00
M1= 0.49500E+00
N1=-0.16399E+00

P2= 0.35900E+00
M2=-0.37900E+00
N2= 0.15410E+01

BP= 0.32001E+00

REACTOR PARAMETERS

OXYGEN CONCENTRATION
URANIUM DIOXIDE CONCENTRATION
GAS FLOW RATE
DILUENT GAS MOLE FRAC
DESIRED CONVERSION
PRESSURE
AMOUNT OF SOLIDS TO BE PROCESSED
TEMPERATURE
RESIDENCE TIME
VOLUME OF REACTOR

CO2= 0.25000E+00 MOLES O2 / MOLES DILUENT GAS
CUO2= 0.13700E-01 MOLES UO2 / KG ZIRCONIUM
G= 0.16700E+01 M**3 / SEC
GAS2= 0.80000E+00
MAX= 0.99900E+00
P= 0.10000E+01 ATM
SS= 0.71400E+03 KG / DAY
T= 0.48000E+03 C
TAU= 0.96771E+03 SEC
V= 0.30000E+00 M**3

DATA POINTS PRIOR TO R.P. = 45
TOTAL NUMBER OF DATA POINTS= 177
REQUIRED TIME FOR DESIRED CONVERSION (SEC) = 0.88200E+05

5	.1216E-01	.2473
.100E+04	.2440E-01	.2473
.150E+04	.3673E-01	.2473
.200E+04	.4914E-01	.2473
.250E+04	.6164E-01	.2473
.300E+04	.7422E-01	.2472
.350E+04	.8690E-01	.2472
.400E+04	.9968E-01	.2472
.450E+04	.1126	.2472
.500E+04	.1255	.2472
.550E+04	.1386	.2471
.600E+04	.1518	.2471
.650E+04	.1691	.2471
.700E+04	.1785	.2471
.750E+04	.1921	.2470
.800E+04	.2057	.2470
.850E+04	.2195	.2470
.900E+04	.2334	.2469
.950E+04	.2475	.2469
.100E+05	.2617	.2469
.105E+05	.2761	.2468
.110E+05	.2906	.2468
.115E+05	.3052	.2468
.120E+05	.3201	.2467
.125E+05	.3351	.2467
.130E+05	.3503	.2467
.135E+05	.3657	.2466
.140E+05	.3813	.2466
.145E+05	.3971	.2465
.150E+05	.4132	.2465
.155E+05	.4295	.2464
.160E+05	.4460	.2464
.165E+05	.4629	.2463
.170E+05	.4800	.2462
.175E+05	.4974	.2462
.180E+05	.5151	.2461
.185E+05	.5332	.2460
.190E+05	.5517	.2459
.195E+05	.5707	.2458
.200E+05	.5900	.2457
.205E+05	.6099	.2456
.210E+05	.6304	.2455
.215E+05	.6515	.2453
.220E+05	.6733	.2451
.225E+05	.6960	.2452
.230E+05	.7169	.2456
.235E+05	.7361	.2460
.240E+05	.7539	.2463
.245E+05	.7703	.2466
.250E+05	.7894	.2468
.255E+05	.7994	.2471
.260E+05	.8123	.2473
.265E+05	.8243	.2475
.270E+05	.8354	.2477
.275E+05	.8457	.2478
.280E+05	.8552	.2480
.285E+05	.8641	.2481
.290E+05	.8723	.2483
.295E+05	.8800	.2484
.300E+05	.8871	.2485
.305E+05	.8938	.2486

.380E+05	.9111	.2489
.325E+05	.9161	.2489
.315E+05	.9289	.2490
.310E+05	.9253	.2491
.340E+05	.9294	.2491
.345E+05	.9332	.2492
.390E+05	.9368	.2492
.355E+05	.9402	.2493
.360E+05	.9434	.2493
.365E+05	.9464	.2494
.370E+05	.9492	.2494
.375E+05	.9518	.2494
.380E+05	.9543	.2495
.385E+05	.9566	.2495
.390E+05	.9588	.2495
.395E+05	.9609	.2496
.400E+05	.9628	.2496
.405E+05	.9647	.2496
.410E+05	.9664	.2496
.415E+05	.9680	.2497
.420E+05	.9696	.2497
.425E+05	.9710	.2497
.430E+05	.9724	.2497
.435E+05	.9737	.2497
.440E+05	.9749	.2497
.445E+05	.9761	.2498
.450E+05	.9772	.2498
.455E+05	.9782	.2498
.460E+05	.9792	.2498
.465E+05	.9801	.2498
.470E+05	.9810	.2498
.475E+05	.9818	.2498
.480E+05	.9826	.2498
.485E+05	.9834	.2498
.490E+05	.9841	.2498
.495E+05	.9848	.2499
.500E+05	.9854	.2499
.505E+05	.9861	.2499
.510E+05	.9866	.2499
.515E+05	.9872	.2499
.520E+05	.9877	.2499
.525E+05	.9882	.2499
.530E+05	.9887	.2499
.535E+05	.9892	.2499
.540E+05	.9896	.2499
.545E+05	.9900	.2499
.550E+05	.9904	.2499
.555E+05	.9908	.2499
.560E+05	.9912	.2499
.565E+05	.9915	.2499
.570E+05	.9918	.2499
.575E+05	.9921	.2499
.580E+05	.9924	.2499
.585E+05	.9927	.2499
.590E+05	.9930	.2499
.595E+05	.9933	.2499
.600E+05	.9935	.2499
.605E+05	.9938	.2499
.610E+05	.9940	.2500
.615E+05	.9942	.2500
.620E+05	.9944	.2500
.625E+05	.9946	.2500
.630E+05	.9948	.2500
.635E+05	.9950	.2500

.645E+05	.9953	.2500
.650E+05	.9955	.2500
.655E+05	.9957	.2500
.660E+05	.9958	.2500
.665E+05	.9959	.2500
.670E+05	.9961	.2500
.675E+05	.9962	.2500
.680E+05	.9963	.2500
.685E+05	.9965	.2500
.690E+05	.9966	.2500
.695E+05	.9967	.2500
.700E+05	.9968	.2500
.705E+05	.9969	.2500
.710E+05	.9970	.2500
.715E+05	.9971	.2500
.720E+05	.9972	.2500
.725E+05	.9973	.2500
.730E+05	.9974	.2500
.735E+05	.9974	.2500
.740E+05	.9975	.2500
.745E+05	.9976	.2500
.750E+05	.9977	.2500
.755E+05	.9977	.2500
.760E+05	.9978	.2500
.765E+05	.9979	.2500
.770E+05	.9979	.2500
.775E+05	.9980	.2500
.780E+05	.9981	.2500
.785E+05	.9981	.2500
.790E+05	.9982	.2500
.795E+05	.9982	.2500
.800E+05	.9983	.2500
.805E+05	.9983	.2500
.810E+05	.9984	.2500
.815E+05	.9984	.2500
.820E+05	.9985	.2500
.825E+05	.9985	.2500
.830E+05	.9985	.2500
.835E+05	.9986	.2500
.840E+05	.9986	.2500
.845E+05	.9987	.2500
.850E+05	.9987	.2500
.855E+05	.9987	.2500
.860E+05	.9988	.2500
.865E+05	.9988	.2500
.870E+05	.9988	.2500
.875E+05	.9989	.2500
.880E+05	.9989	.2500