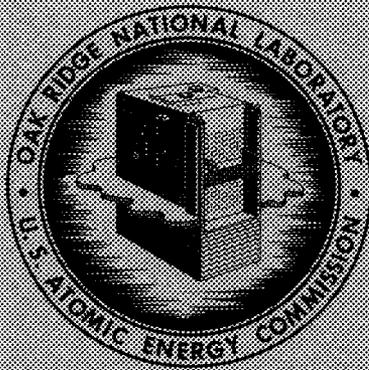


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ANALYSIS OF UO_2 DISSOLUTION IN
NITRIC ACID SOLUTION

H. F. Johnson



OAK RIDGE NATIONAL LABORATORY

operated by

UNION CARBIDE CORPORATION

for the

U. S. ATOMIC ENERGY COMMISSION

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H. F. Johnson
Consultant
Unit Operations Section

DATE ISSUED

SEP 4 1962

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee
operated by
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U. S. Atomic Energy Commission

ABSTRACT

A model assuming a zero-order reaction and dependence of specific area, a , on fraction of pellets dissolved, F , is proposed to explain the dissolution of UO_2 pellets in nitric acid solution. A Fortran program for the IBM-7090 was developed to calculate the rate coefficient, k_a , and F from experimental data for concentration as a function of time obtained in countercurrent stage runs. Application of the Fortran program to data from eight experimental runs led to fairly good agreement between the k_a -vs- F relations for all stages of the eight runs. The average relation for all runs can be represented by a second-order polynomial. From the k_a -vs- F polynomial and the zero-order reaction model, an analog computer representation of the multistage dissolution process was developed and applied for conditions of the eight experimental runs. The concentration profiles thus calculated were in very good agreement with the original experimental profiles. The studies covered conditions of initial acid concentrations from 5.5 to 8.0 M and L/V ratios from 0.126 to 0.223 min^{-1} .

The model described here should be tested with other systems. It is desirable that the sampling time interval be decreased relative to the dissolution rate. Thus for rates of the magnitude studied here, more frequent sampling should be used. However for slower rates, the 10-min interval is probably satisfactory. If intervals other than 10 min are used, the Fortran program will have to be modified.

CONTENTS

	<u>Page</u>
1.0 Introduction	1
2.0 Equipment Operation	1
3.0 Mathematical Model	4
4.0 Calculation of k_a from Experimental Data	5
5.0 Application of k_a -vs- F Relation	27

1.0 INTRODUCTION

The purpose of this work was to develop a relatively simple mathematical model which can, with a limited number of bench-scale experimental data, predict performance of a full-scale countercurrent stage dissolver.

Dissolution of spent fuel elements from power reactors is a key step in fuel processing. There is a great need for a sound method of designing such dissolving processes and for predicting the behavior of a given system in existing equipment. Dissolution characteristics vary widely from one type of fuel element to another and from one dissolvent to another. The work described here deals with dissolution of UO_2 pellets in nitric acid solution. The method developed will not necessarily apply to other types of fuel elements or other acids, but will have to be tested for the cases of interest.

Experimental work used in the report was performed in the Unit Operations Section by B. C. Finney.

2.0 EQUIPMENT OPERATION

In the operation of the continuous-spiral pellet dissolver (Fig. 1), fresh acid is fed continuously to the upper end of the dissolver. The acid overflows successively from one compartment to the next, the compartments being contained between adjacent elements of the spiral. The pellets to be dissolved are fed to the lower end of the dissolver. The spiral rotates in a direction such as to carry the solid pellets upward through the dissolver. Thus, each batch of pellets moves through the dissolver countercurrently to the acid flow.

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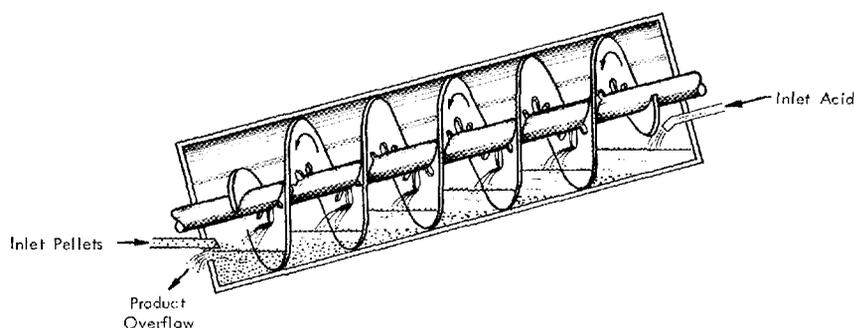


Fig. 1. Continuous spiral pellet dissolver.

The startup operation is shown schematically in terms of an equivalent bucket operation in Fig. 2. Fresh acid enters the battery (diagram a) and flows from one stage to the next, down to stage 1, where a batch of pellets is introduced at zero time. Stage 1 then moves up the battery. Fresh acid overflows from the stage ahead into stage 1, and the spent solution, containing dissolved solute and spent acid, overflows from stage 1.

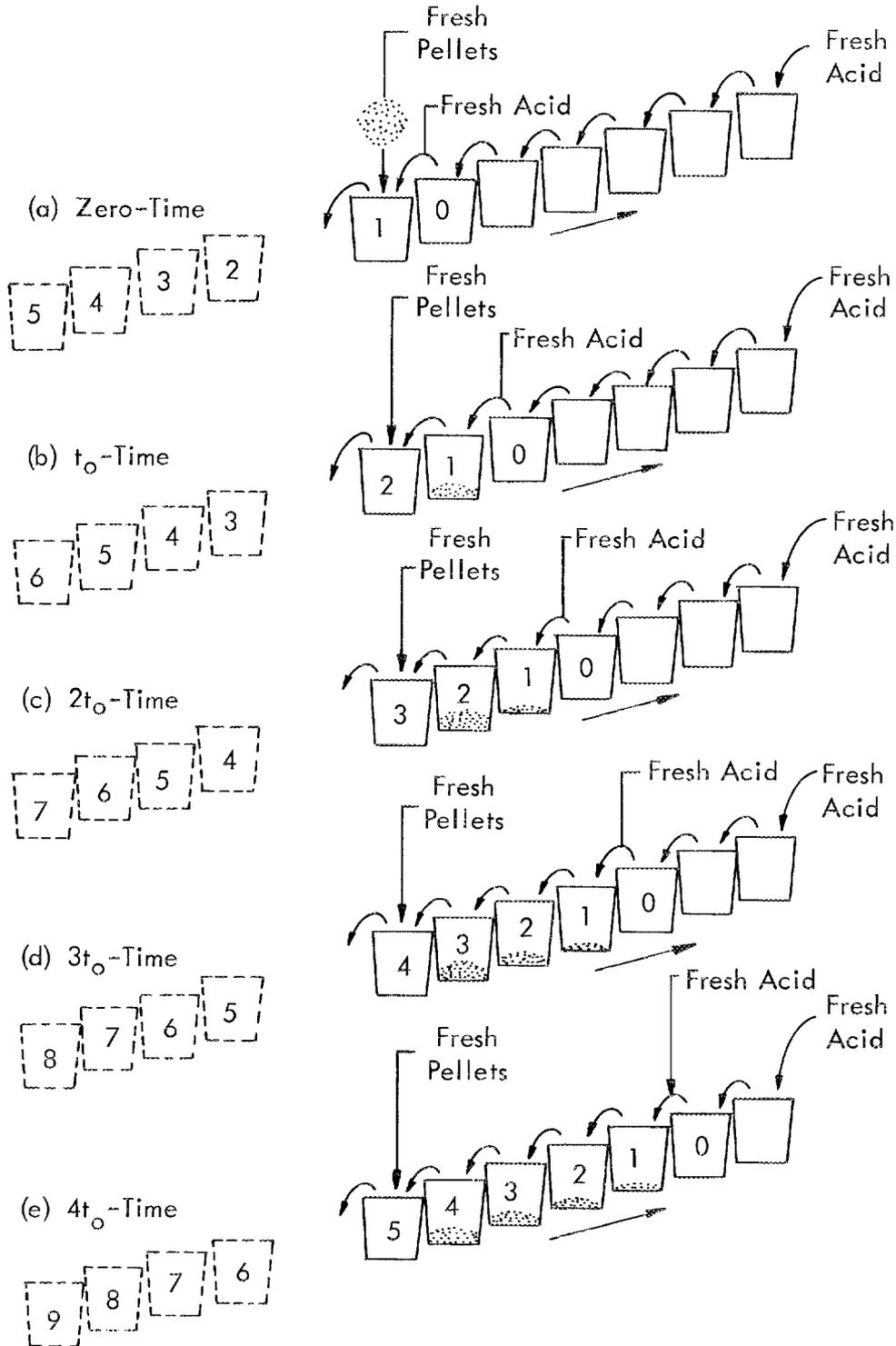


Fig. 2. Startup of dissolver in terms of equivalent bucket operation.

If the spiral requires t_0 time to make one complete revolution, we may treat the system as if a batch of fresh pellets is introduced to stage 2 at time t_0 . At this instant (diagram b), the effluent from stage 1 is introduced to stage 2 as feed solution.

Stages 1 and 2 move up the battery and at time $2t_0$ (diagram c), a batch of fresh pellets is introduced to stage 3 and overflow solution from stage 2 is fed to stage 3. The sequence continues, with a new stage being introduced at each time interval, t_0 .

At zero time the concentration of dissolved pellets in stage 1 is zero (Fig. 3), but it rises rapidly to a maximum and then drops off to zero as complete dissolution of the pellets is approached. At t_0 time the concentration in stage 2 is the same as that in the effluent from stage 1 at this instant. Again, the concentration rises to a maximum and drops to zero as complete dissolution of pellets of stage 2 is approached. This behavior continues for the succeeding stages, and as steady state is approached, the curves from one stage to the next become identical in shape and magnitude.

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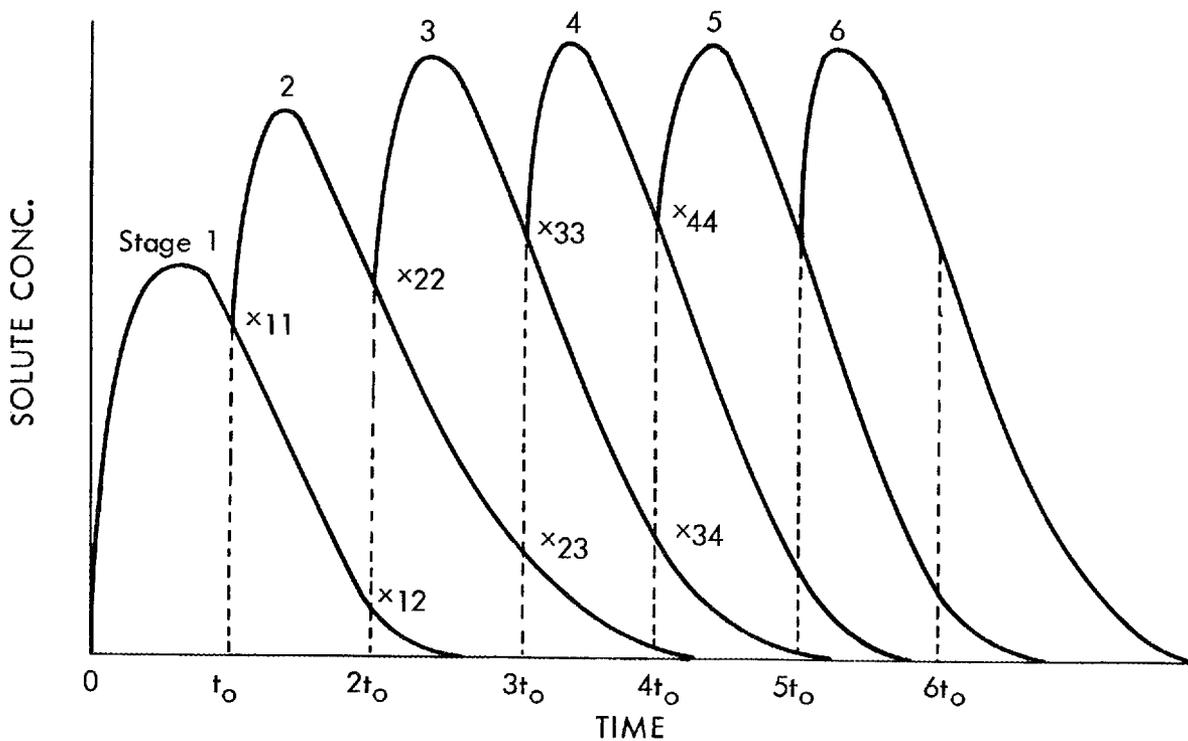


Fig. 3. Typical concentration - time behavior of dissolved pellets.

3.0 MATHEMATICAL MODEL

Consider the nth stage of the dissolution operation (Fig. 4). If V is the total volume of the stage, liters, m_n is the mass of the solid, g, being dissolved (UO_2 in terms of uranium content, in this case); and ρ is the density (mass of uranium in UO_2 per solid volume, in this case) of the solid, g/liter, then $(V - m_n/\rho)$ is the volume of the solution. It will be assumed that each stage is well mixed and the solute concentration, C_n in grams per liter, is therefore uniform throughout stage n. Thus $[C_n(V - m_n/\rho)]$ is the instantaneous solute (dissolved uranium) content of the nth stage. Let L be the solution flow rate, in liters per minute, here assumed constant with time and unchanged between inlet and outlet flow for each stage. An overall instantaneous solute material balance gives

$$-\frac{d [C_n (V - \frac{m_n}{\rho})]}{dt} = LC_n - LC_{n-1} - r_n \left(V - \frac{m_n}{\rho} \right) \quad (1)$$

where t is the time in minutes, and r is the rate of dissolution of solid per unit volume of solution, g/min.liter, or

$$r_n = - \frac{d m_n / dt}{V - m_n / \rho} \quad (2)$$

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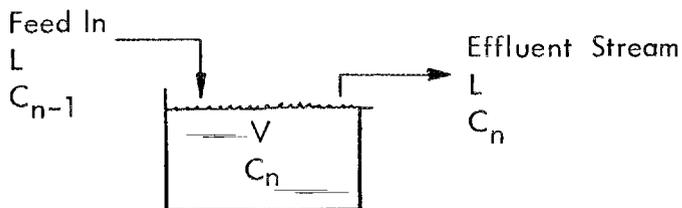


Fig. 4. Conditions of nth stage.

The kinetic mechanism assumed will be that of a zero order reaction, i.e. the dissolution rate is independent of solute concentration in the solution. The rate should, however, be proportional to the area of the solid exposed to the solution. Thus

$$r_n = \frac{kam_n}{V - \frac{m_n}{\rho}} \quad (3)$$

where k is a specific rate constant, rate per unit area of solid, g/min.cm², and "a" is the effective solid surface per unit mass of solid, cm²/g. For a given dissolution it will be assumed that k is constant since dissolution

will be carried out in a boiling solution and temperature will change relatively little. The neglecting of possible effects of acid concentration will have to be justified experimentally. The specific surface, a , is assumed to be a function of the fraction of the solids dissolved, F , because the solids probably tend to crumble and expose increased surface to the solution as the dissolution proceeds. There is no convenient means for separating area and absolute rate effects; thus k_a will be treated as a single term.

An assumption that leads to considerable simplification of the above equations is that m/ρ is very small relative to V . This assumption is not strictly valid for the experimental conditions studied because the volume of the pellets fed to each stage is a significant fraction of the total stage volume. However, the assumption will be made because the experimental data scatter extensively and the refinement of allowing for pellet volume is probably not justified in light of the additional complexity introduced to the problem. Omitting the m/ρ terms from eqs. 1, 2, and 3 leads to

$$-V \frac{dc_n}{dt} = LC_n - LC_{n-1} - Vr_n \quad (4)$$

$$r_n = -\frac{1}{V} \frac{dm_n}{dt} \quad (5)$$

$$r_n = \frac{1}{V} k_a m_n \quad (6)$$

4.0 CALCULATION OF k_a FROM EXPERIMENTAL DATA

Data from a series of bench-scale runs on the dissolution of UO_2 pellets in nitric acid were reported by B. C. Finney in Unit Operations Section Monthly Progress Reports, February 1961 (CF 61-2-65), March 1961 (CF 61-3-67), April 1961 (ORNL-TM-32), and May 1961 (ORNL-TM-33). In each run, a series of beakers was each charged with ~600 g of UO_2 . Nitric acid solution was fed at a constant rate to the first beaker, overflow from this beaker was sampled at 10-min intervals, and, after an hour, was directed to the second beaker. Overflow from this was sampled at 10-min intervals and after another hour was diverted to the third beaker. This sequence was repeated for six to nine beakers. Thus the behavior of the beakers simulated the behavior of stages in a continuous dissolver whose rate of revolution is one cycle per hour. The fresh nitric acid concentration, constant in each run, ranged from 5.5 to 8.0 M (Table 1). The data were plotted in Figs. 5 through 12, where the lower sets of dotted lines represent smoothed experimental uranium concentrations vs time data. Points at 10-min intervals were read from these curves and used in computing instantaneous values of k_a .

Since point data are to be used, the above differential equations are approximated by difference relations. If i is a time index and the differences between successive values denote 10-min intervals, by use of second differences it can be shown that, approximately,

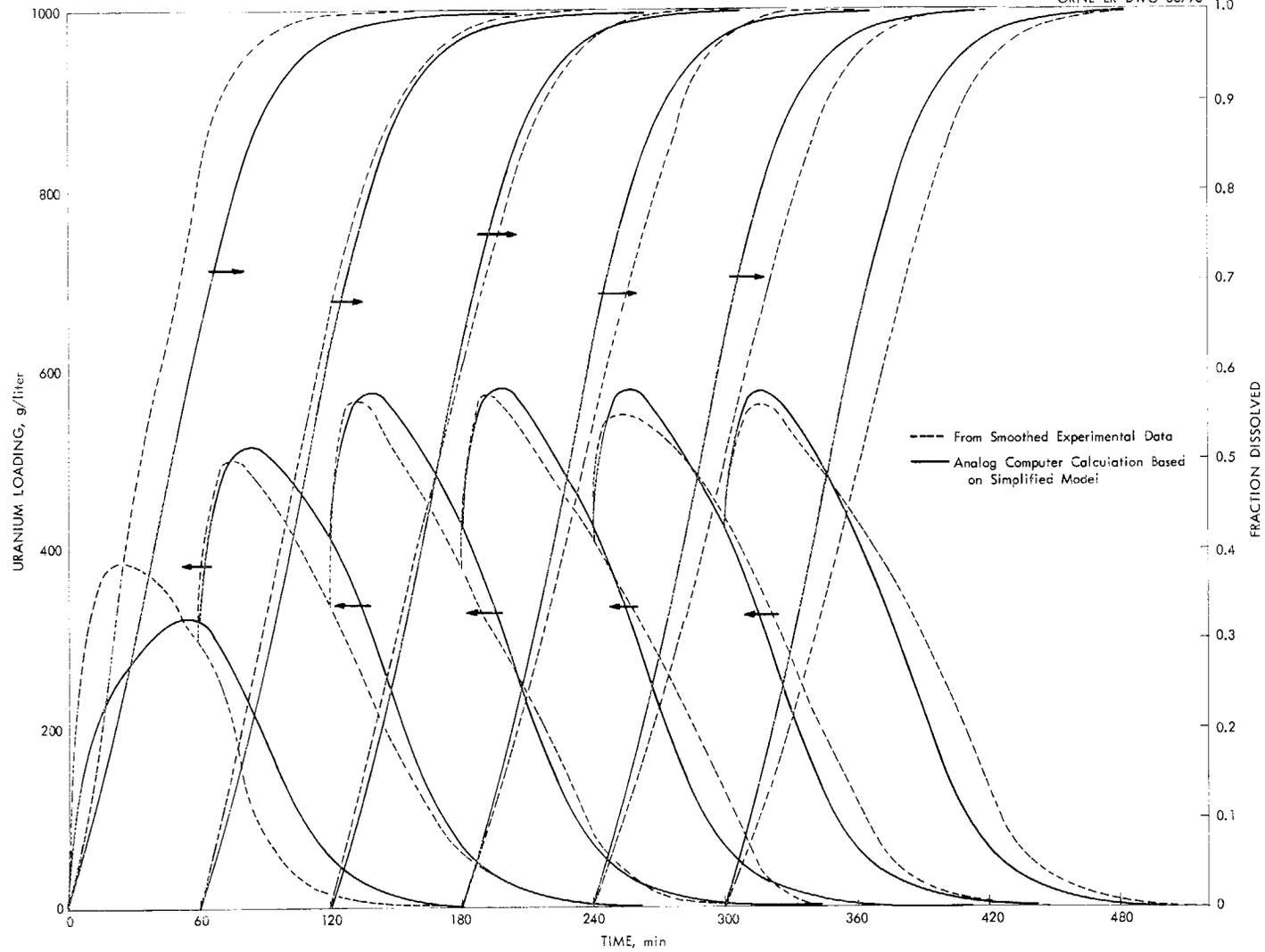


Fig. 5. Case 1, Run R-14; $L/V = 0.126$.

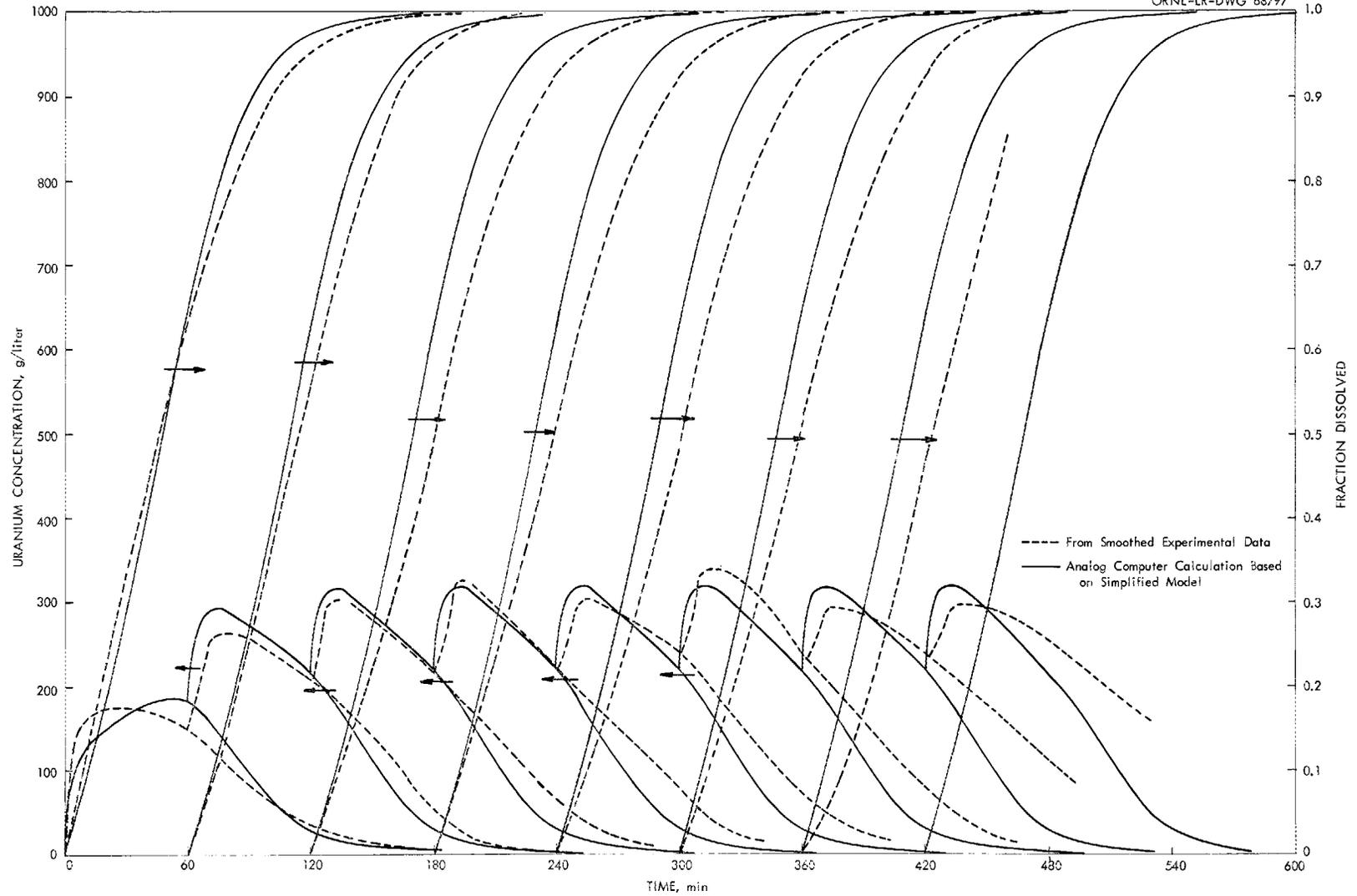


Fig. 6. Case 2, Run R-20; $L/V = 0.223$.

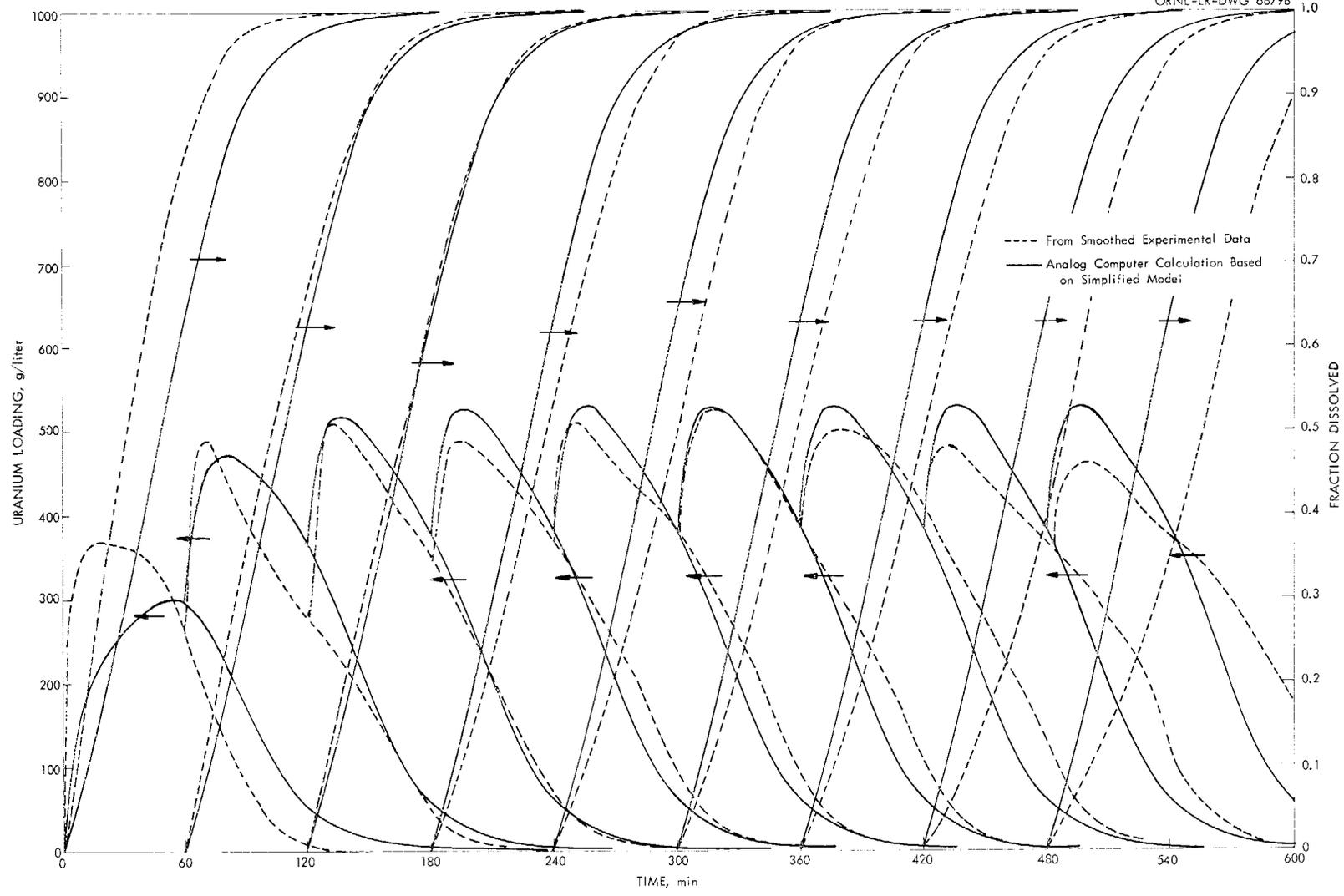


Fig. 7. Case 3, Run R-17; $L/V = 0.137$.

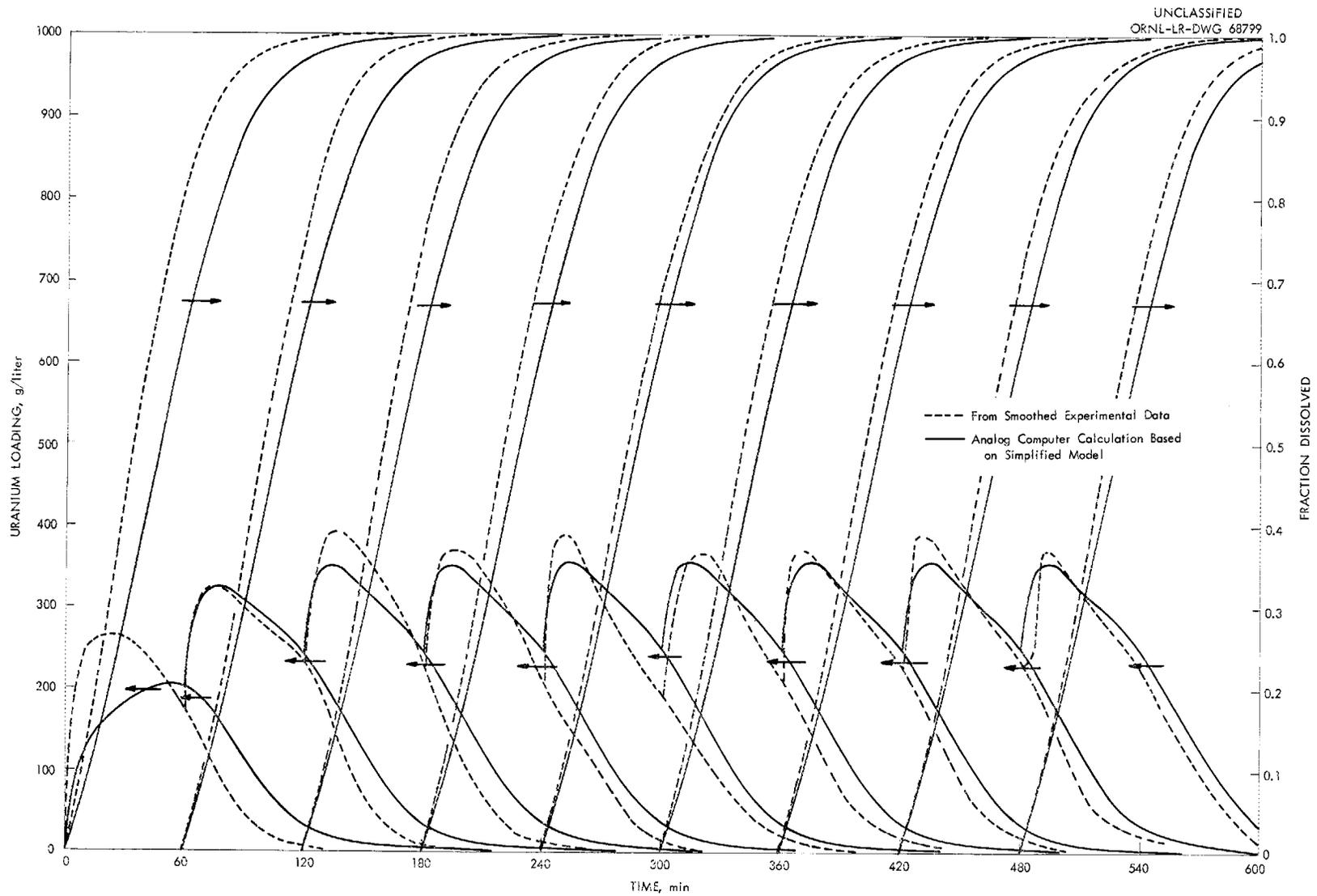


Fig. 8. Case 4, Run R-21; $L/V = 0.202$.

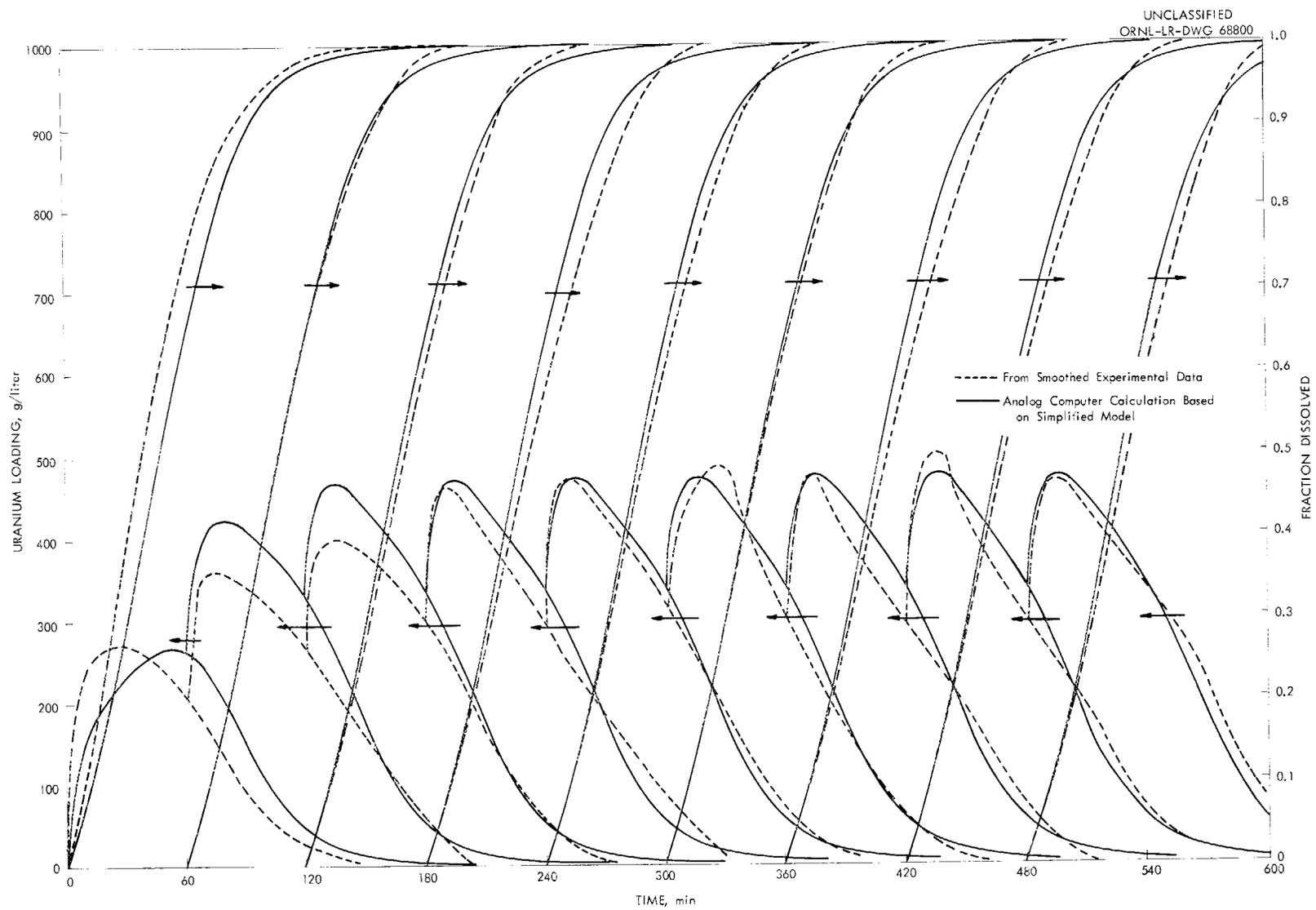


Fig. 9. Case 5, Run R-23; $L/V = 0.153$.

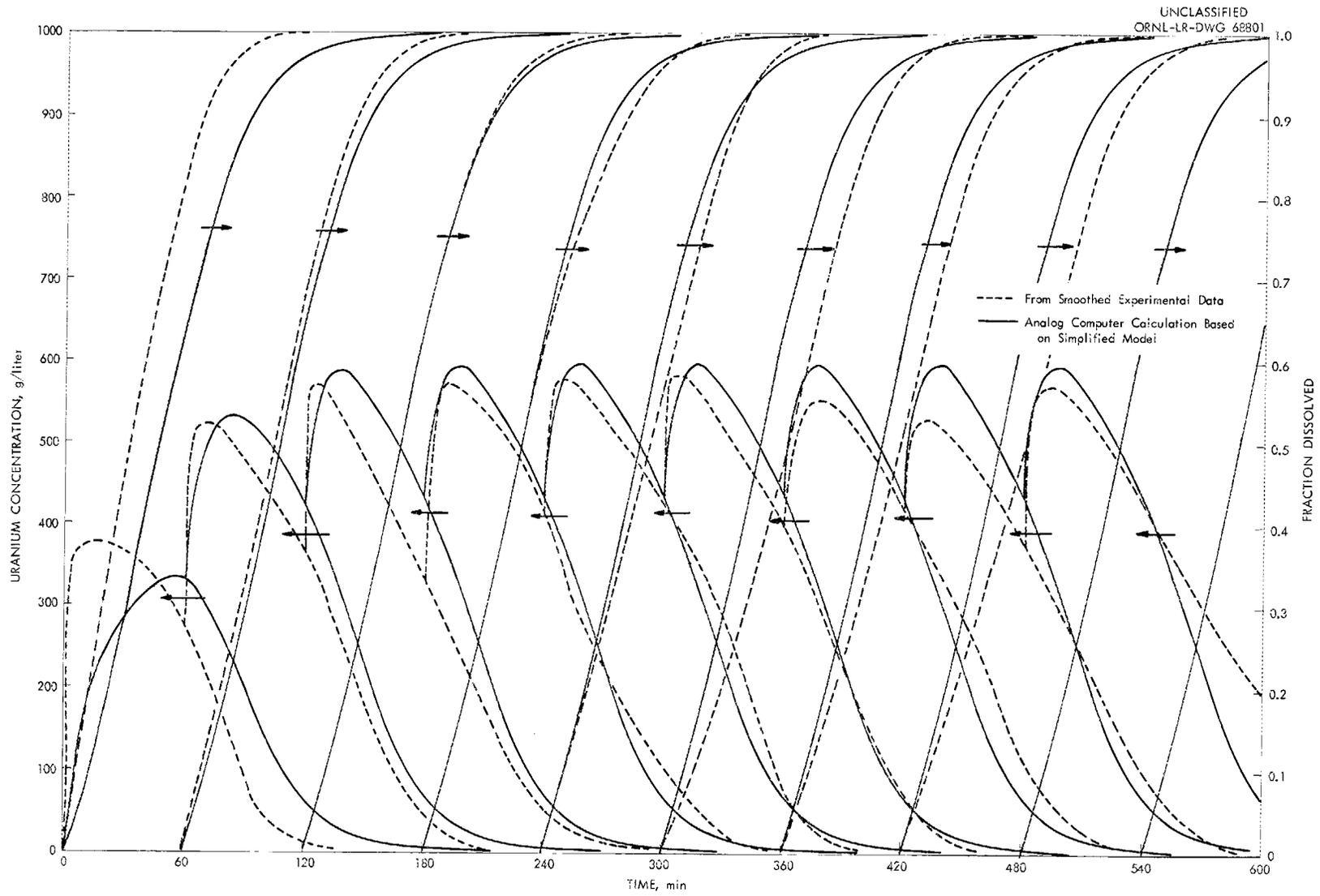


Fig. 10. Case 6, Run R-26; $L/V = 0.122$.

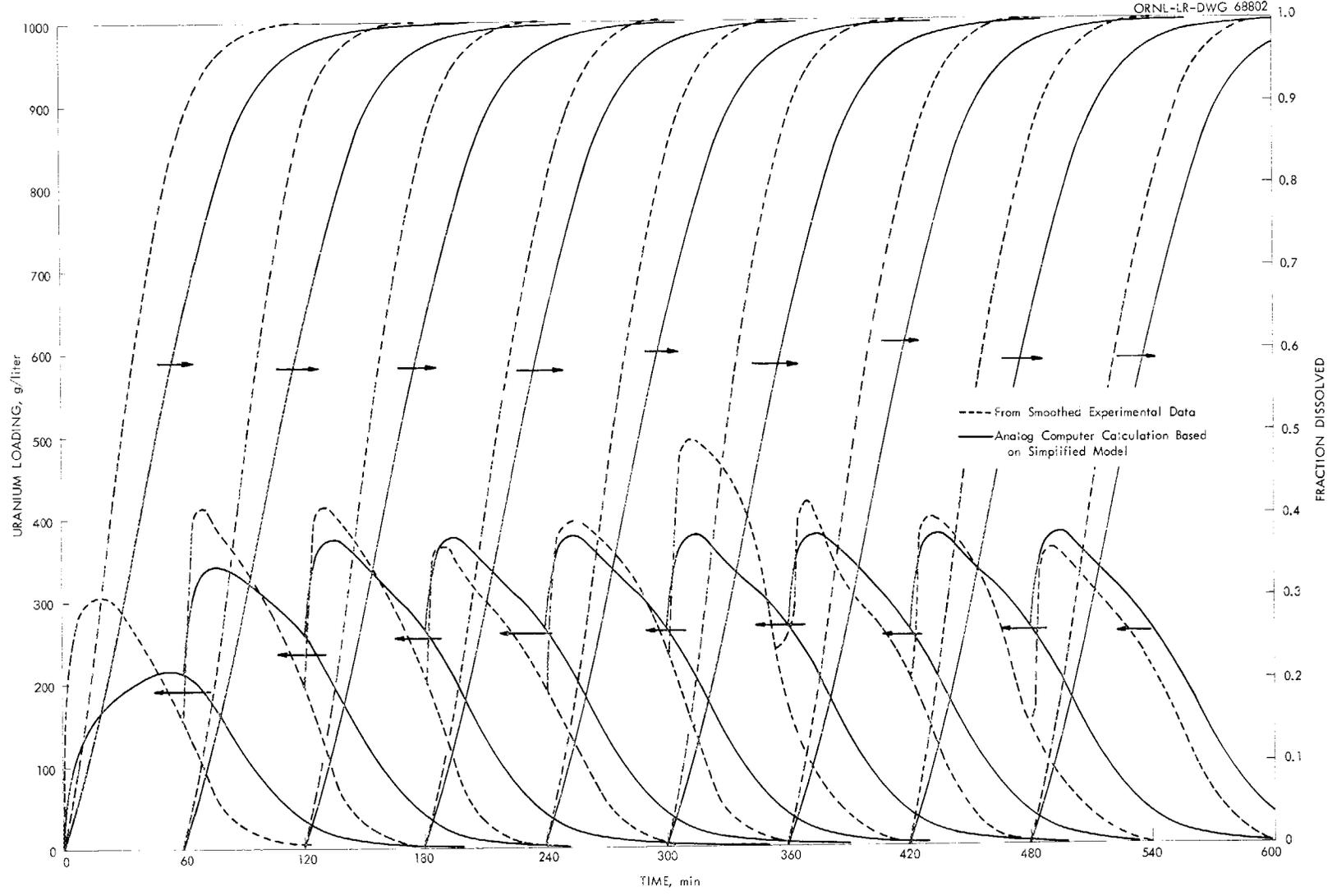


Fig. 11. Case 7, Run R-27; $L/V = 0.190$.

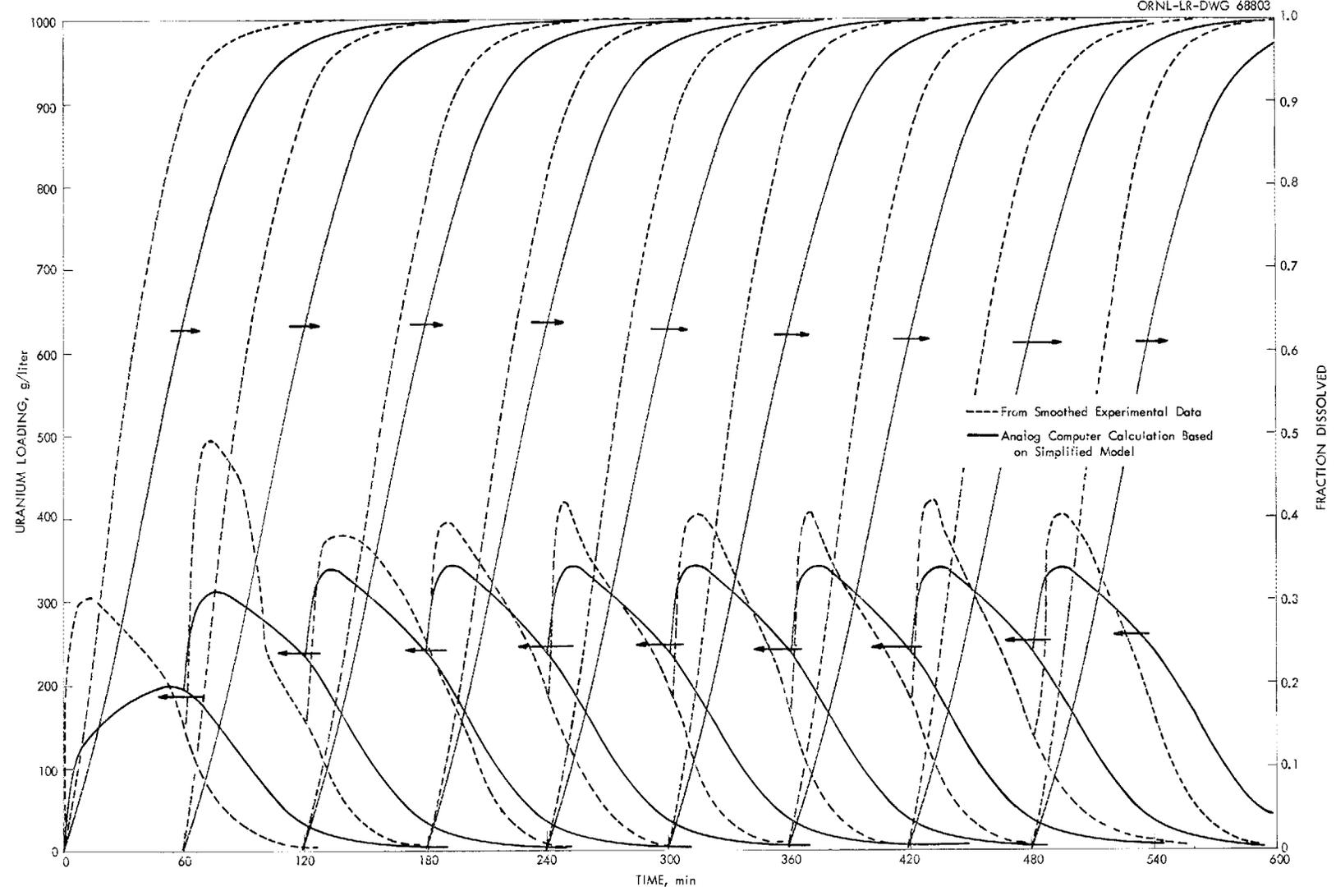


Fig. 12. Case 8, Run R-24; $L/V = 0.208$ (crushed pellets).

Table 1. Summary of Run Conditions

V = 0.150 liter

Computer Case No.	Run No.	Original HNO ₃ Conc., <u>M</u>	Flow Rate (L), liters/min	L/V, min ⁻¹
1	R-14	7.0	0.0189	0.126
2	R-20	5.5	0.0334	0.223
3	R-17	7.0	0.0206	0.137
4	R-21	7.0	0.0303	0.202
5	R-23	7.0	0.0229	0.153
6	R-26	8.0	0.0183	0.122
7	R-27	8.0	0.0285	0.190
8	R-24 ^a	7.0	0.0312	0.208

^aCrushed pellets were used in run R-24, whole pellets in others.

$$\frac{dc_{n,i}}{dt} = \frac{1}{10} (-1.5 c_{n,i} + 2c_{n,(i+1)} - 0.5 c_{n,(i+2)}) \quad (7)$$

Substitution of eq. 7 in eq. 4 and solution for r leads to

$$r_{n,i} = \frac{L}{V} (c_{n,i} - c_{(n-1),i}) + \frac{1}{10} (-1.5 c_{n,i} + 2.0 c_{n,(i+1)} - 0.5 c_{n,(i+2)}) \quad (8)$$

From eq. 5, it is seen that

$$m_0 - m_n = V \int_0^t r_n dt \quad (9)$$

where m_0 is the mass of uranium in the initial charge. By Simpson's "one-third" rule,

$$\text{Uncorrected } (m_0 - m_{n,i}) = \frac{1}{3} (10)V \left[(r_{n,1} + 4r_{n,2} + r_{n,3}) + (r_{n,3} + 4r_{n,4} + r_{n,5}) + \dots + (r_{n,i-2} + 4r_{n,i-1} + r_{n,i}) \right] \quad (10)$$

As i becomes large, $m_{n,i}$ approaches zero. Thus the value of the right-hand side of eq. 10 should approach m_0 for large values of i . In actual practice, experimental errors and approximations in the calculation prevent this condition from being exactly satisfied. One can therefore define

$$C = \frac{m_o}{\lim_{i \rightarrow \text{large value}} [\text{uncorrected } (m_o - m_{n,i})]} \quad (11)$$

On multiplying elements of the right-hand side of eq. 10 by C, one obtains corrected values of $(m_o - m_{n,i})$. The fraction dissolved may be calculated from

$$F_{n,i} = (m_o - m_{n,i})m_o \quad (12)$$

The rate term, ka , is calculated from eq. 6:

$$ka_{n,i} = \frac{V r_{n,i}}{m_o - (m_o - m_{n,i})} \quad (13)$$

A Fortran program for the IBM-7090 was prepared for computation of $r_{n,i}$, $F_{n,i}$, and $ka_{n,i}$ from concentration data by use of eqs. 8, 10-13 (Table 2). Data from the eight runs were processed by this program and the results plotted (Figs. 13 through 20). The shape of the curve for ka vs fraction dissolved, F , is generally the same for all stages of each run, but there is some scatter from stage to stage of any one run. The curve for the first stage is frequently in poor agreement with those of the other stages. This is probably due in part to the very sharp concentration peak that is characteristic of the first stages and to the fact that the 10-min time interval used in the analysis is large relative to these peaks. Hence the dC/dt terms calculated by difference methods are probably in serious error. Also, in most of the runs scatter appears to be worse between stages at F values of 0.75 and higher. This scatter is not surprising because with high F values concentrations are low, and the calculations involve differences between very small numbers, each of whose relative error is large.

The original nitric acid concentrations used in the various runs are shown in Table 1. The nitric acid concentration history for all stages of all runs is reported in the aforementioned progress reports. In attempts to correlate ka with acid concentration for each stage of all runs, no significant trend could be detected. It was concluded that within the acid concentration range of this work and within the accuracy of the experimental work and mathematical analysis, ka is independent of acid concentration.

In Fig. 21 are shown curves, each of which represents the average ka -vs- F relation for all stages of one run. In Fig. 22 the solid line shows the average relation of ka -vs- F for all runs. This curve was fitted by a second-order polynomial, the constants being determined by the method of least squares. The resulting equation

$$ka = 0.007968 + 0.017365 F + 0.028125 F^2 \quad (14)$$

is shown as a dotted line in Fig. 22.

Table 2. Fortran Program^a

```

C      HFJOHNSONSPECIFICAREAFUNCTION,FELLETDISOLUTION      00000001
      DIMENSIONCN(21),CNL1(21),RATE(21),BATCH(21),DIS(21),FRAC(21),AF(21)00000002
      1) 00000003
1 READINPUTTAPE10,2,KASE,NOSTA,N,L,FOV,V,BATCHO 00000004
2 FORMAT(I3/I3/I3/I1/(E10.4)) 00000005
  READINPUTTAPE10,3,(CN(I),I=1,N) 00000006
3 FORMAT(E10.4) 00000007
  READINPUTTAPE10,3,(CNL1(I),I=1,N) 00000008
  N1=N-2 00000009
  DO5I=1,N1 00000010
5 RATE(I)=(-1.5*CN(I)+2.*CN(I+1)-0.5*CN(I+2))/10.+FOV*(CN(I)-CNL1(I))00000011
  1) 00000012
  SUM=0. 00000013
  DO6I=3,N1,2 00000014
6 SUM=SUM+3.3*V*(RATE(I-2)+4.*RATE(I-1)+RATE(I)) 00000015
  C=BATCHO/SUM 00000016
  DIS(1)=0. 00000017
  DO8I=3,N1,2 00000018
8 DIS(I)=DIS(I-2)+3.3*V*(RATE(I-2)+4.*RATE(I-1)+RATE(I))*C 00000019
  DO9I=1,N1,2 000000190
  FRAC(I)=DIS(I)/BATCHO 00000020
9 AF(I)=V*RATE(I)/(BATCHO-DIS(I)) 00000021
  WRITEOUTPUTTAPE9,10,KASE,NOSTA 00000022
10 FORMAT(I1H0//16H CASE NUMBERI3,17H STAGE NUMBERI3//51H 00000023
  1 RATE FRACTION DISSOLVED AREA FUNCTION/) 00000024
  DO12I=1,N1,2 00000001
  WRITEOUTPUTTAPE9,11,RATE(I),FRAC(I),AF(I) 00000002
11 FORMAT(E15.4,E16.4,E19.4) 00000003
12 CONTINUE 00000004
  IF(I-L)1,14,1 00000005
14 CALLEXIT 00000006
  END(1,1,0,0,1,0,0,0,0,0,0,0,0,0,0,0)

```

^aThe Fortran code words or letters have the following meanings:

KASE	Case No.	I	Subscript i
NOSTA	Stage No.	CN	C_n
N	No. of concentration values (N must be odd)	CNL 1	C_{n-1}
L	0 if not last case of last stage; 1 if last case of last stage	RATE	r
FOV	L/V	SUM	Uncorrected $(m_0 - m_{n,i})$
V	V	C	Correction Factor
BATCHO	m_0	DIS(I)	$(m_0 - m_{n,i})$ corrected
		FRAC	Fraction dissolved, F
		AF(I)	$ka_{n,i}$

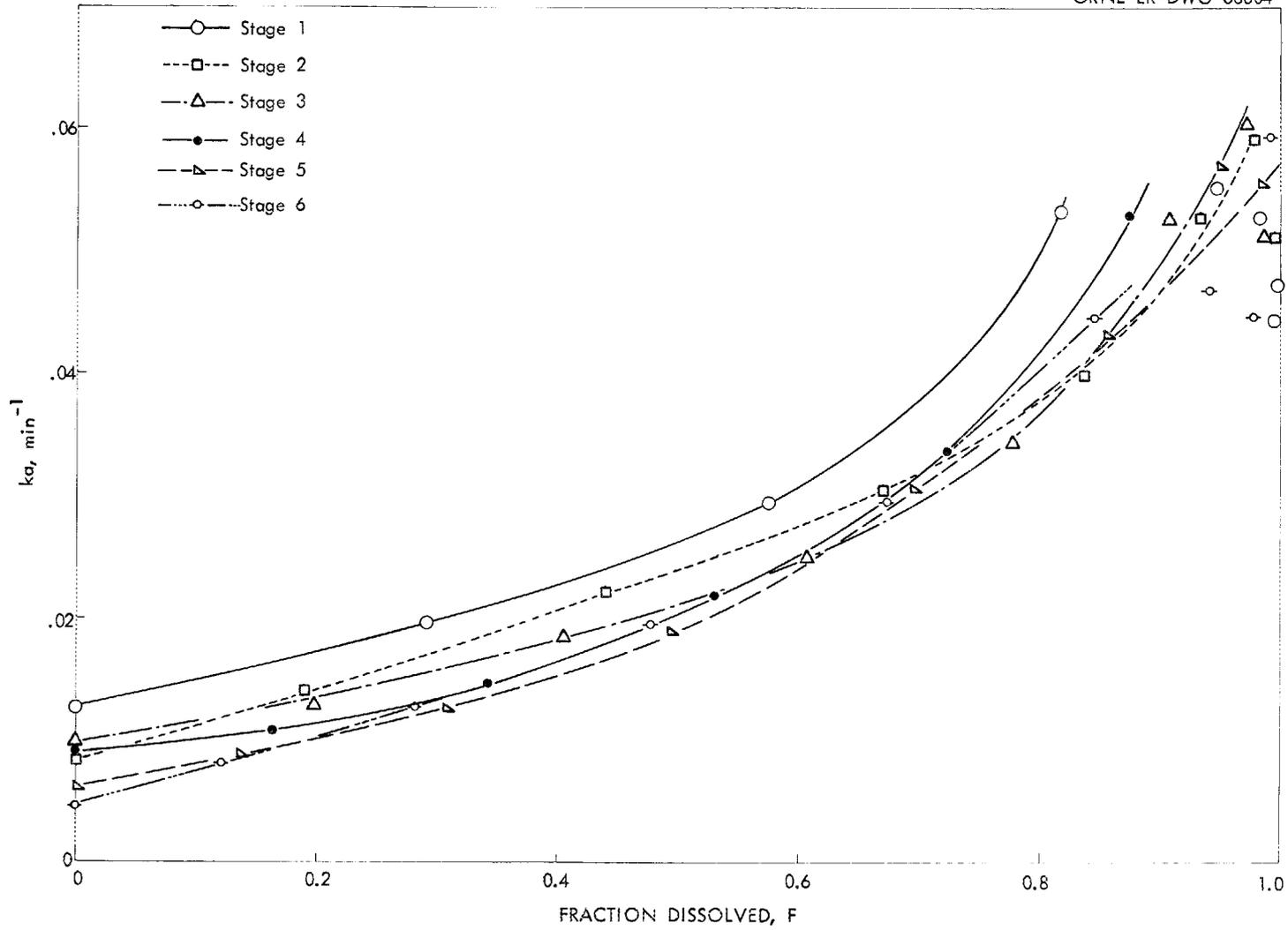


Fig. 13. ka vs. fraction of UO_2 pellets dissolved for all stages of Run R-14, computer case 1 ($L/V = 0.126 \text{ min}^{-1}$).

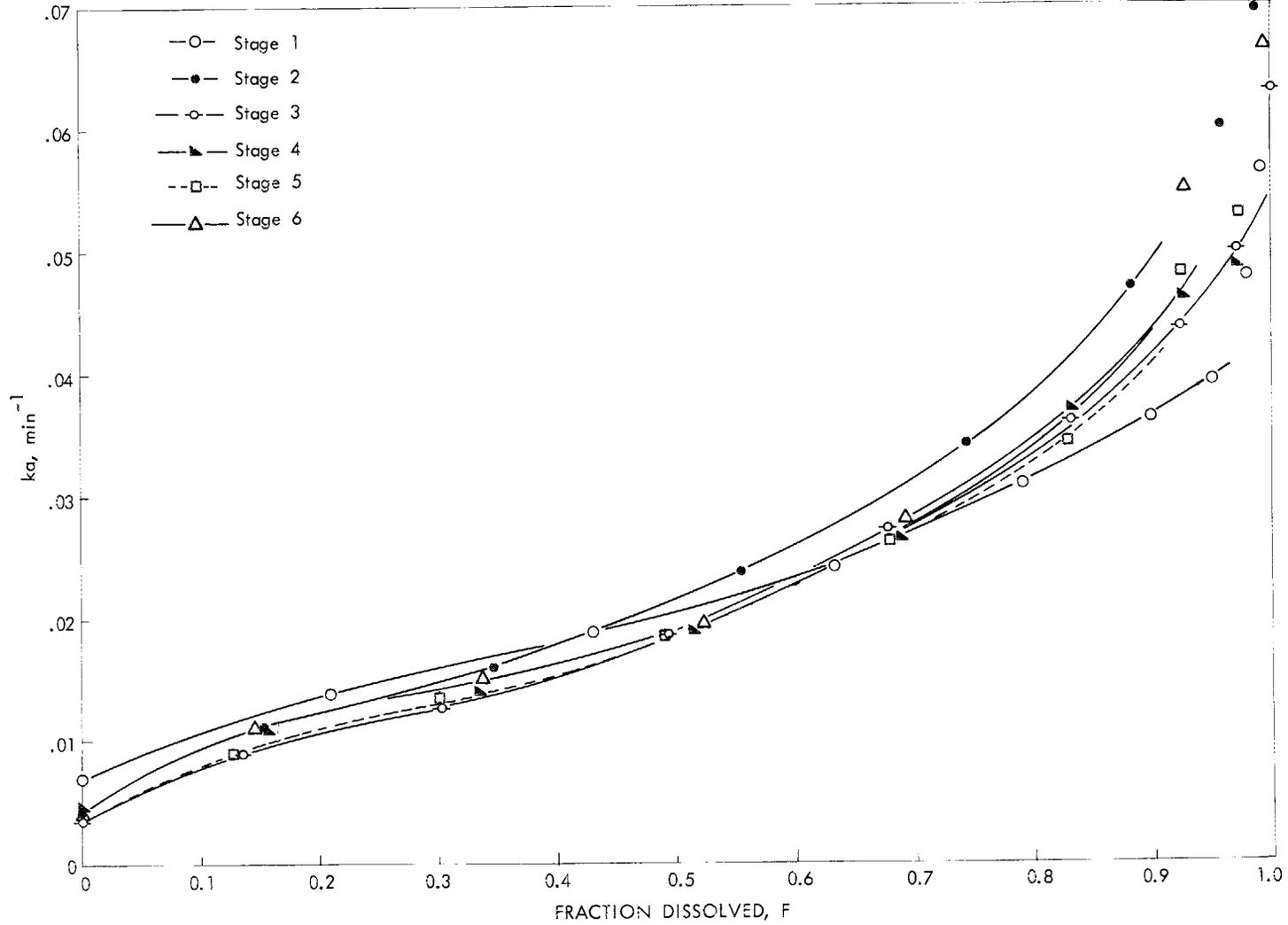


Fig. 14. k_a vs. fraction UO_2 pellets dissolved for all stages of Run R-20, computer case 2 ($L/V = 0.223 \text{ min}^{-1}$).

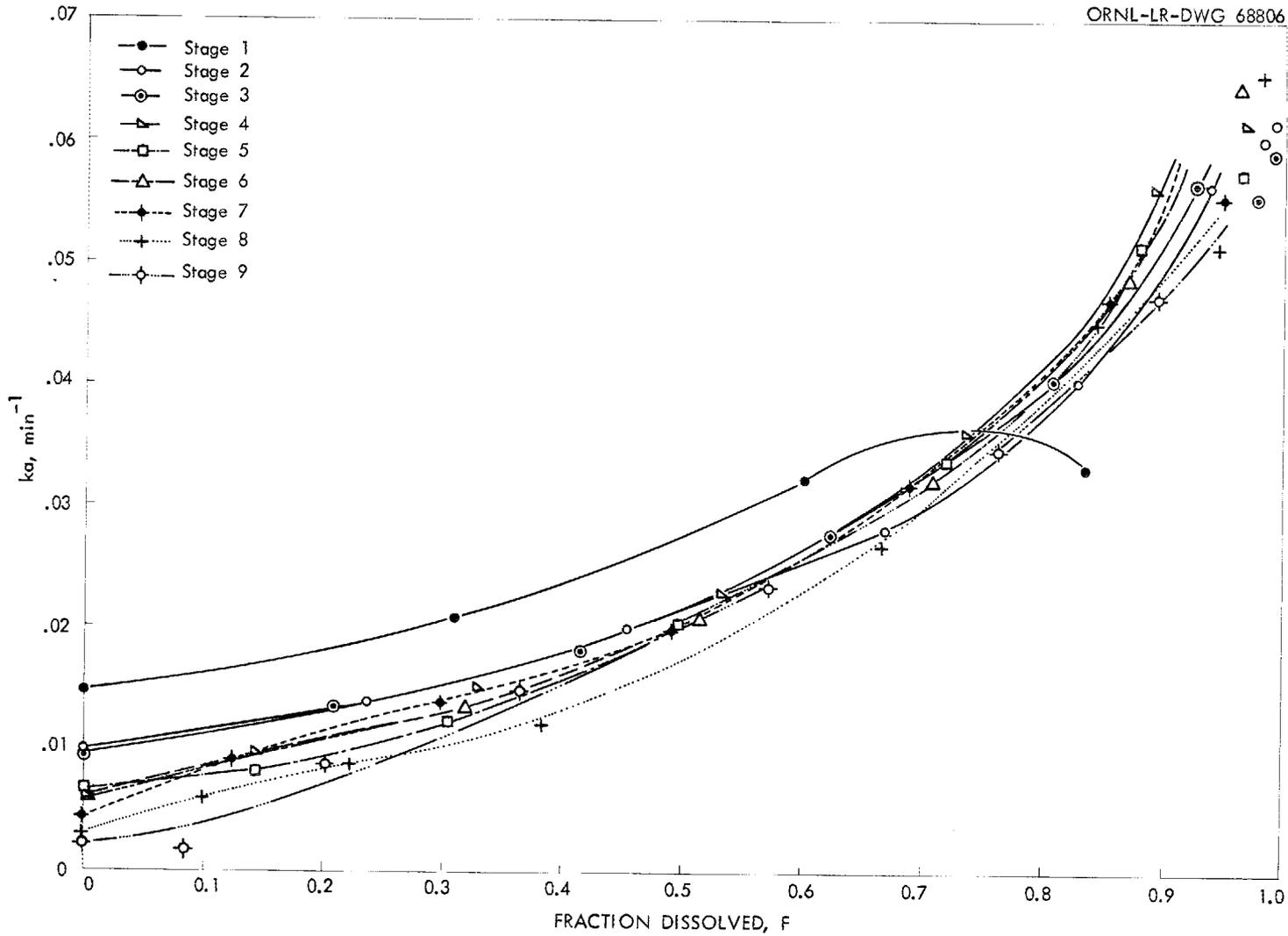


Fig. 15. ka vs. fraction UO_2 pellets dissolved for all stages of Run R-17, computer case 3 ($L/V = 0.137 \text{ min}^{-1}$).

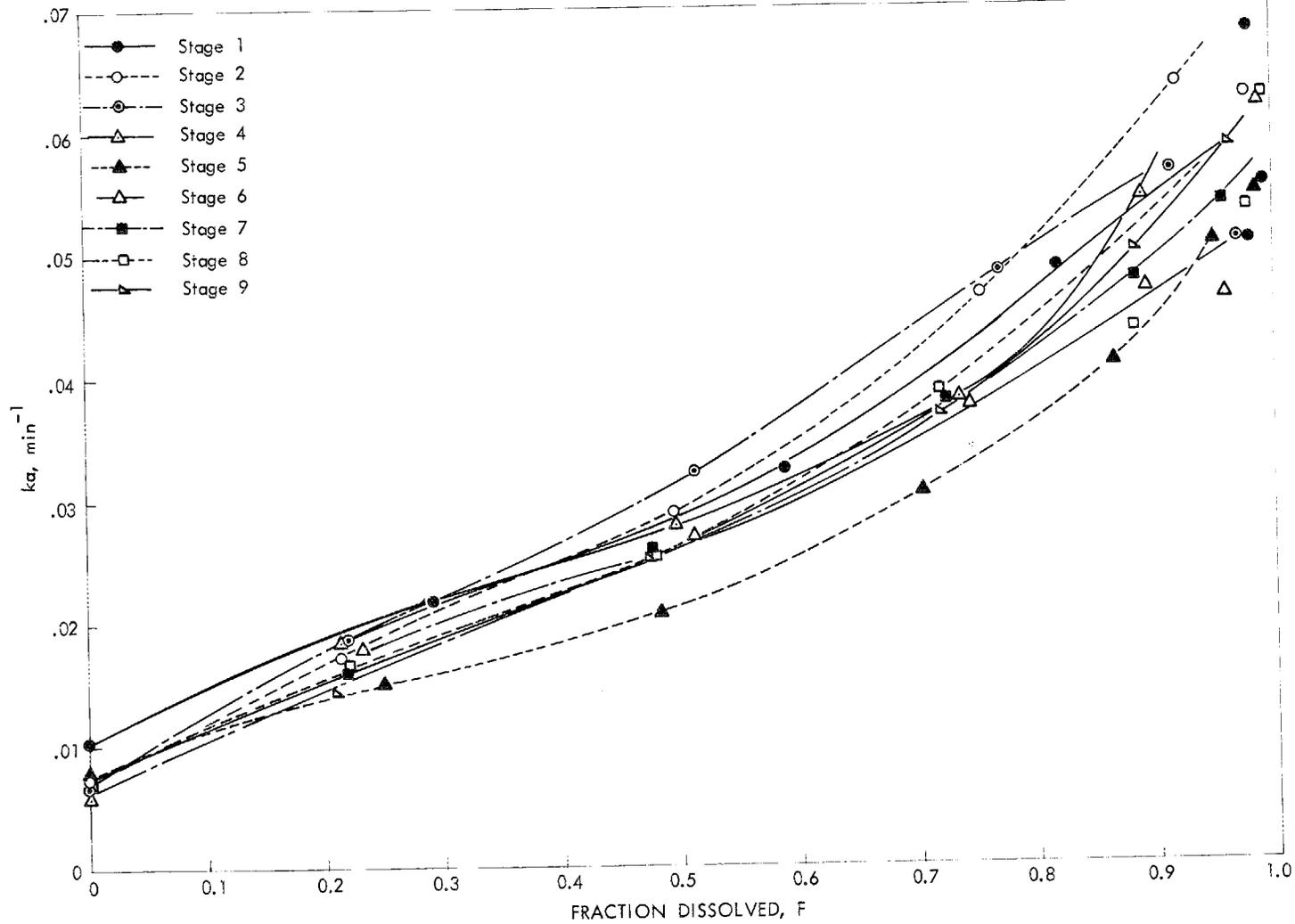


Fig. 16. k_a vs. fraction UO_2 pellets dissolved for all stages of Run R-21, computer case 4 ($L/V = 0.202 \text{ min}^{-1}$).

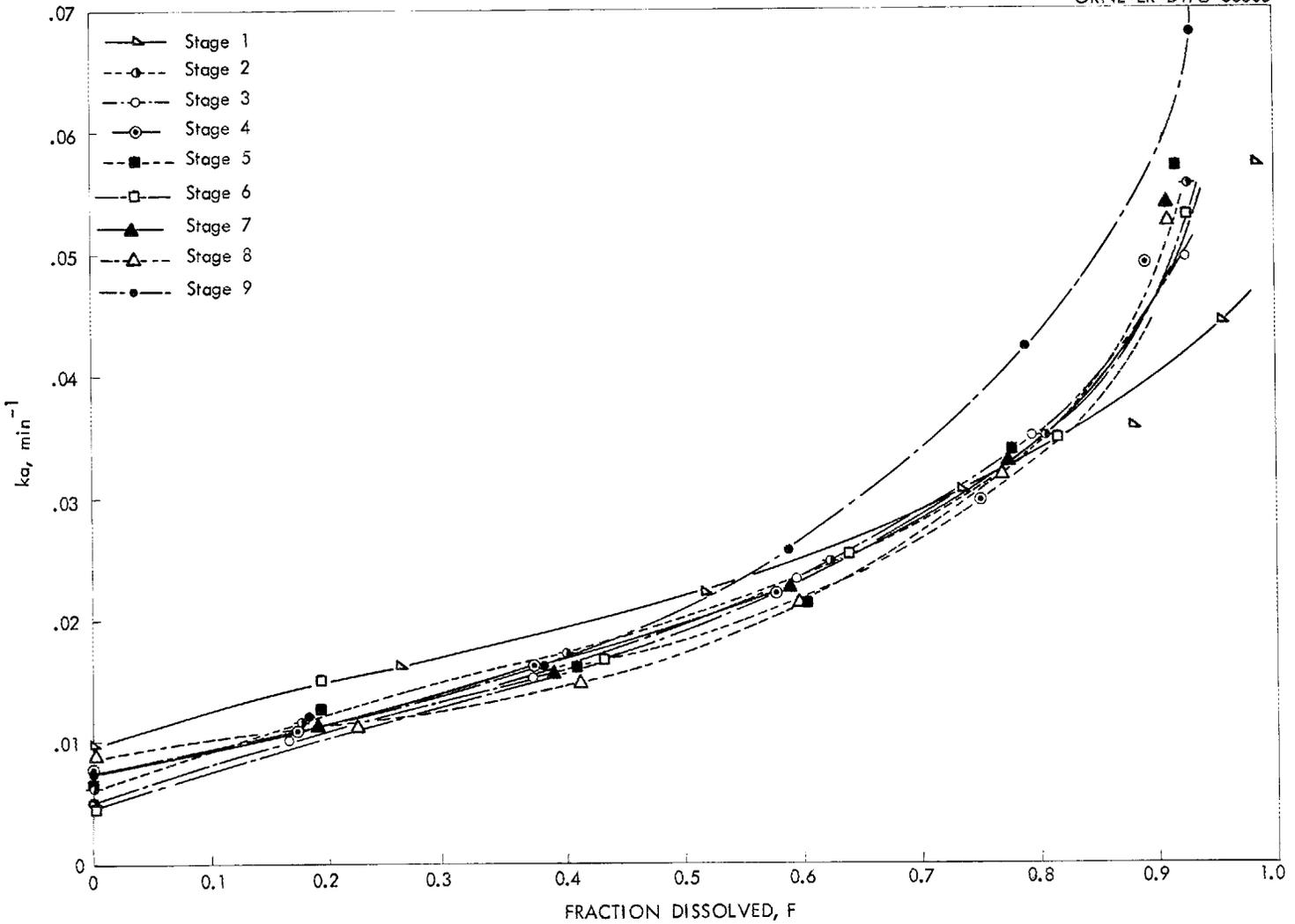


Fig. 17. k_a vs. fraction UO_2 pellets dissolved for all stages of Run R-23, computer case 5 ($L/V = 0.153 \text{ min}^{-1}$).

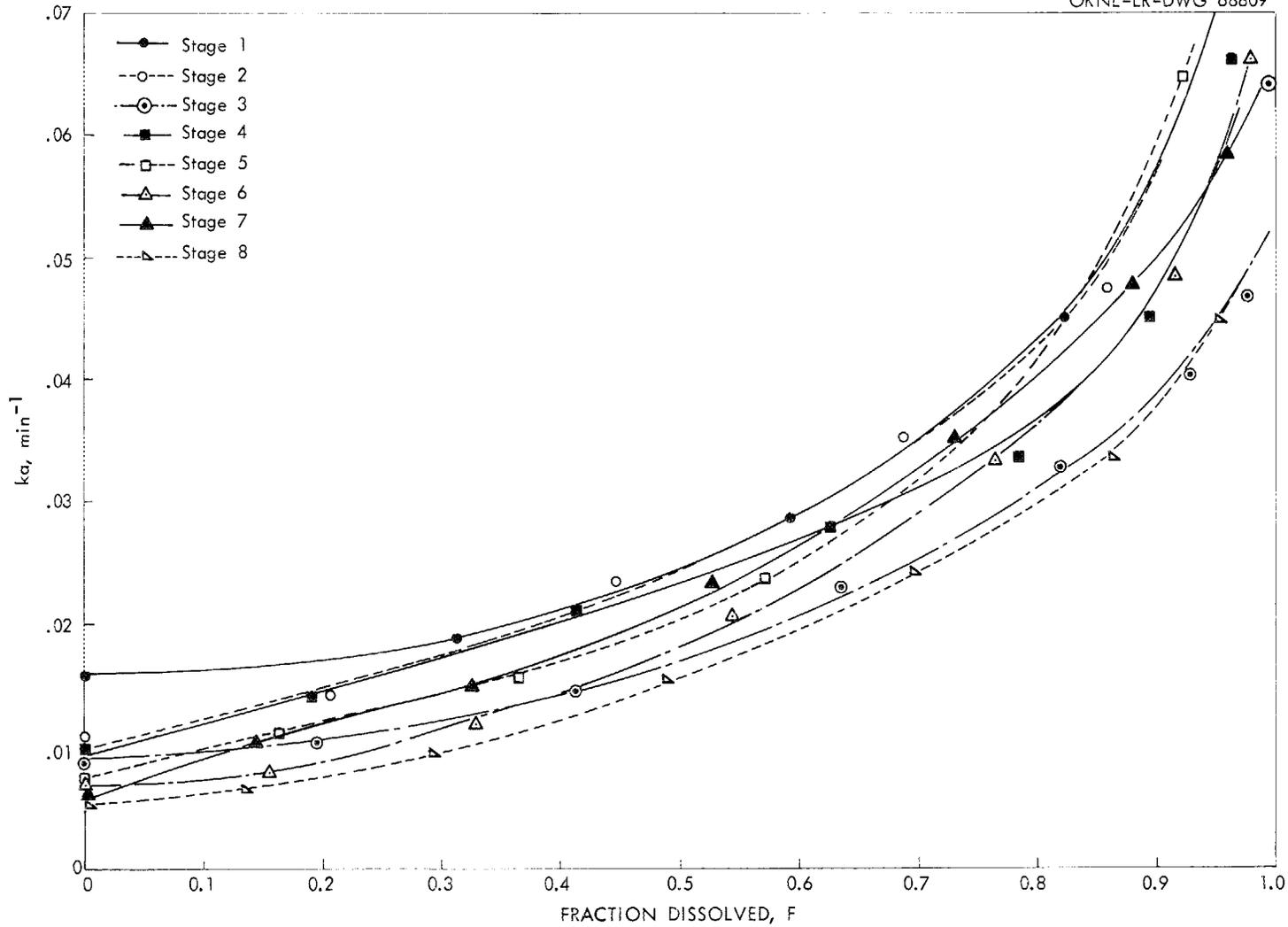


Fig. 18. ka vs. fraction UO_2 pellets dissolved for all stages of Run R-26, computer case 6 ($L/V = 0.122 \text{ min}^{-1}$).

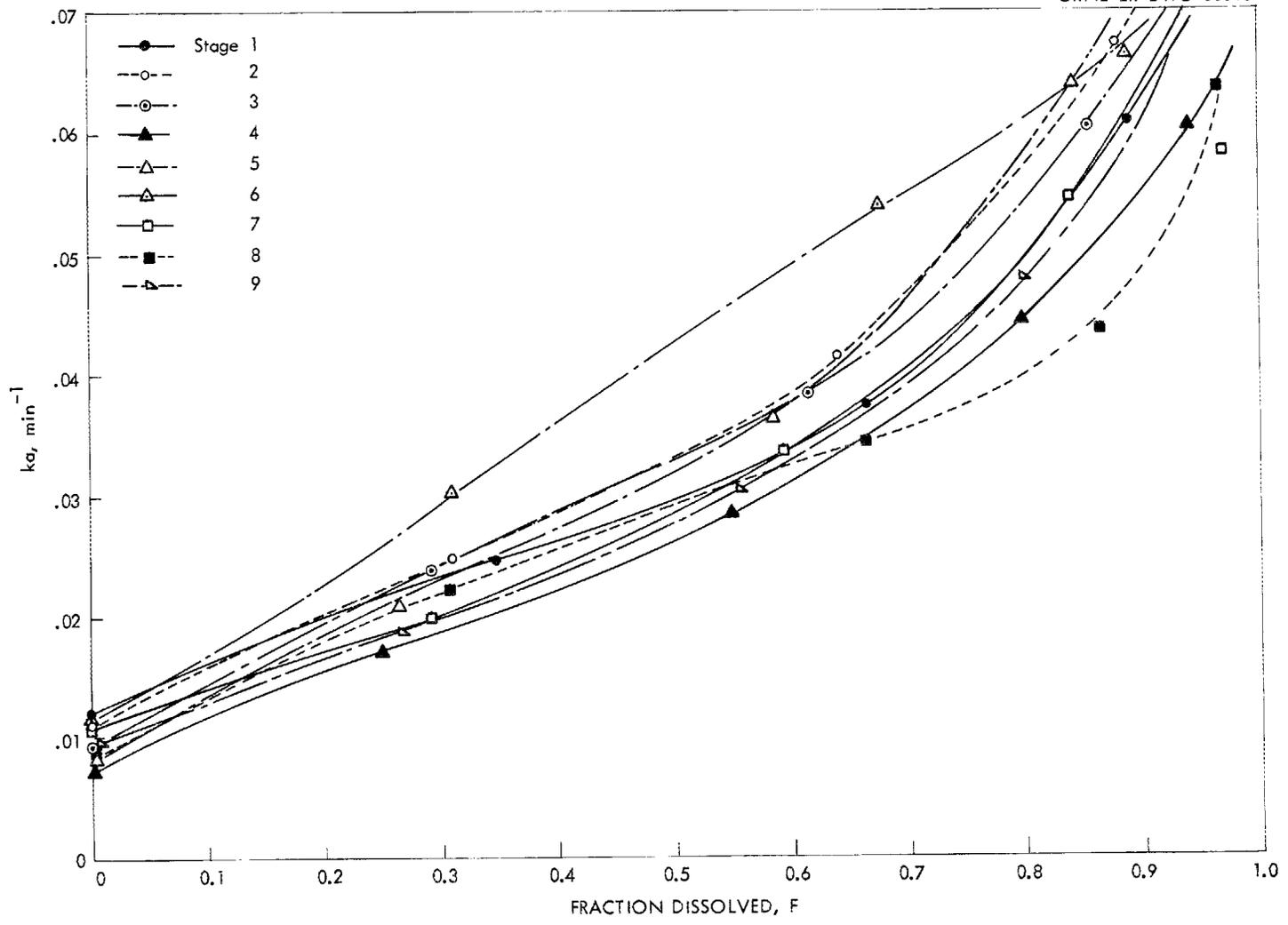


Fig. 19. ka vs. fraction UO_2 crushed pellets dissolved for all stages of Run R-27, computer case 7 ($L/V = 0.190 \text{ min}^{-1}$).

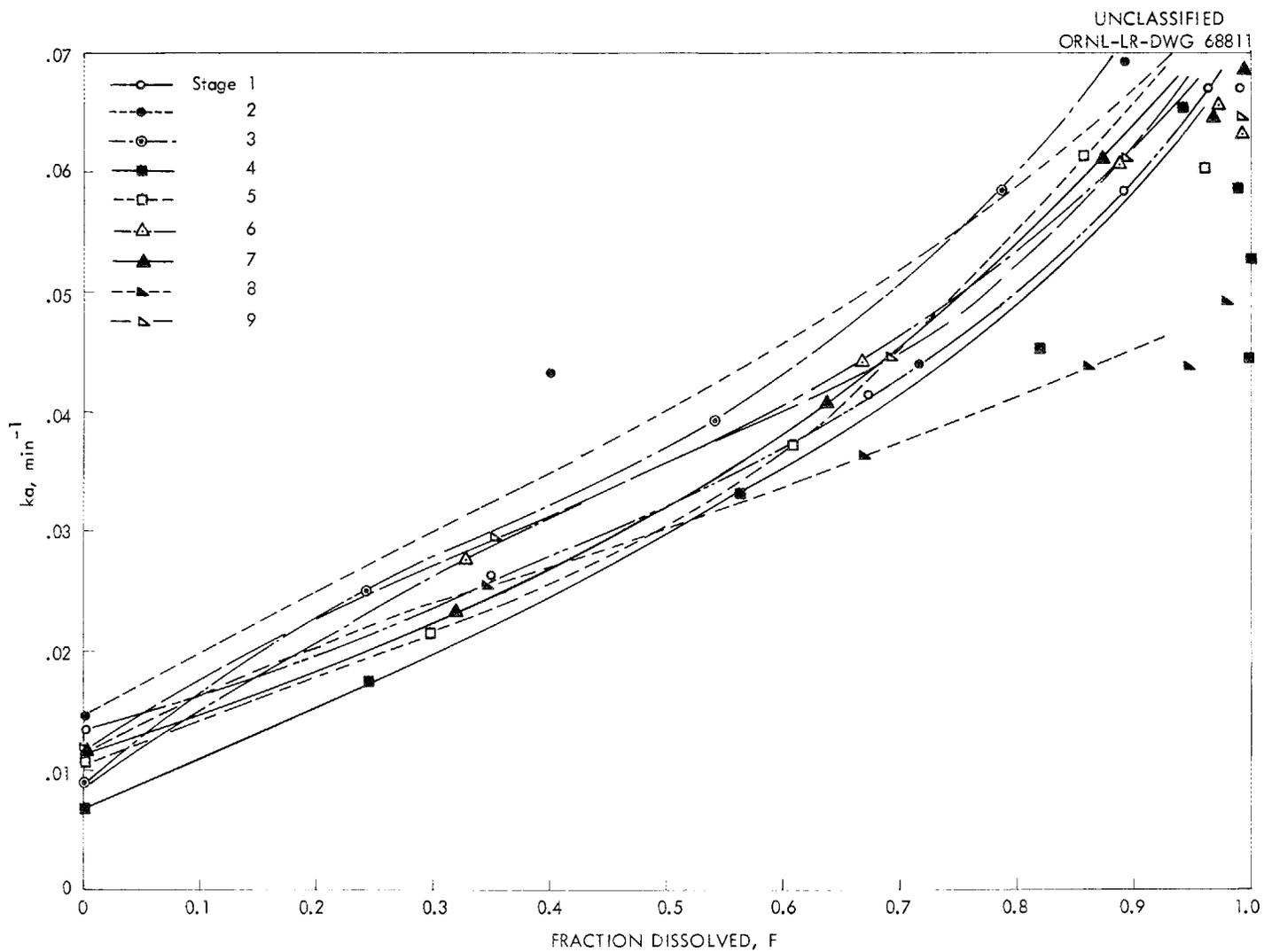


Fig. 20. k_a vs. fraction UO_2 crushed pellets dissolved for all stages of Run R-24, computer case 8 ($L/V = 0.208 \text{ min}^{-1}$).

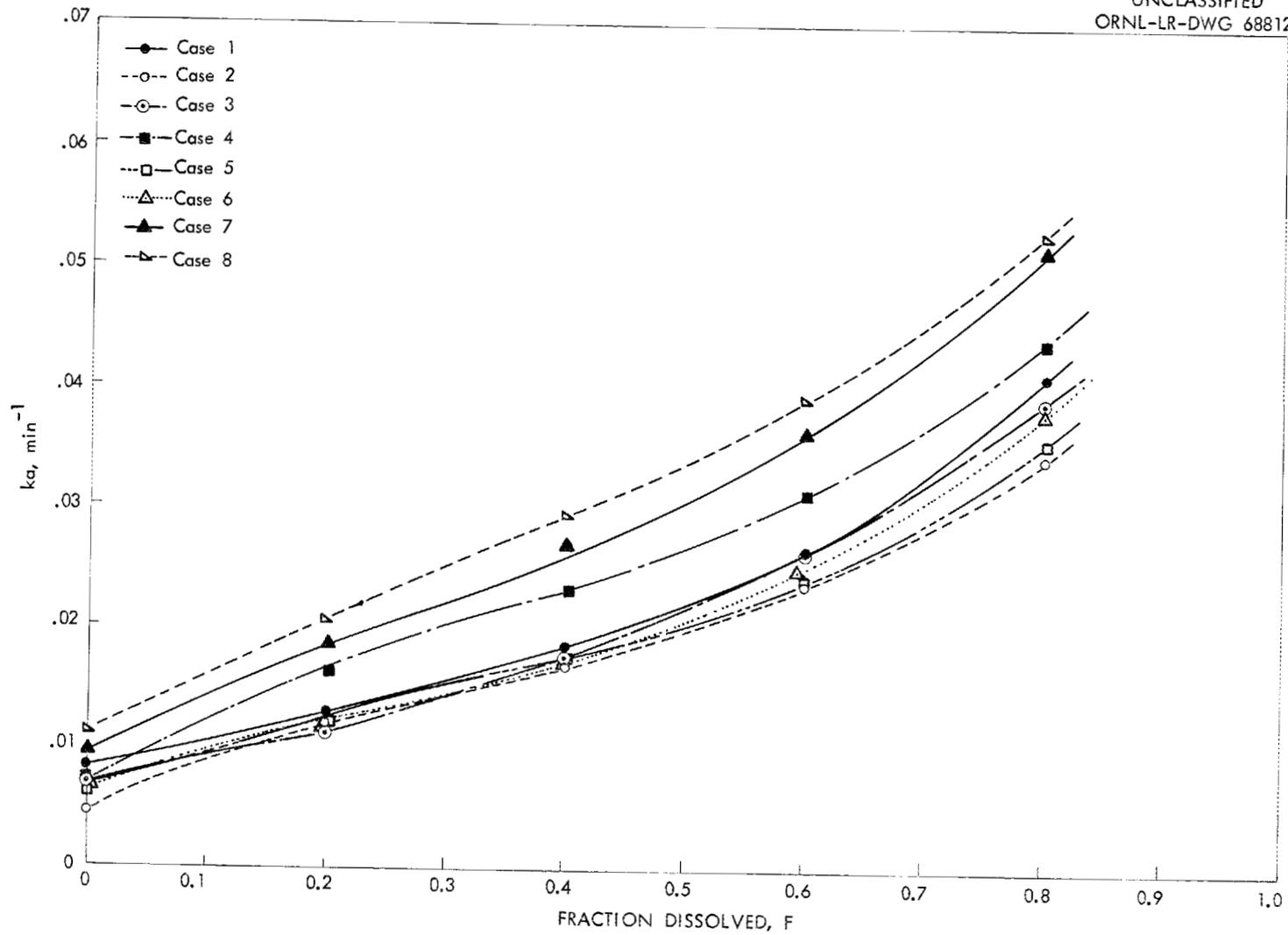


Fig. 21. Average k_a for all stages of each run vs. fraction UO_2 dissolved.

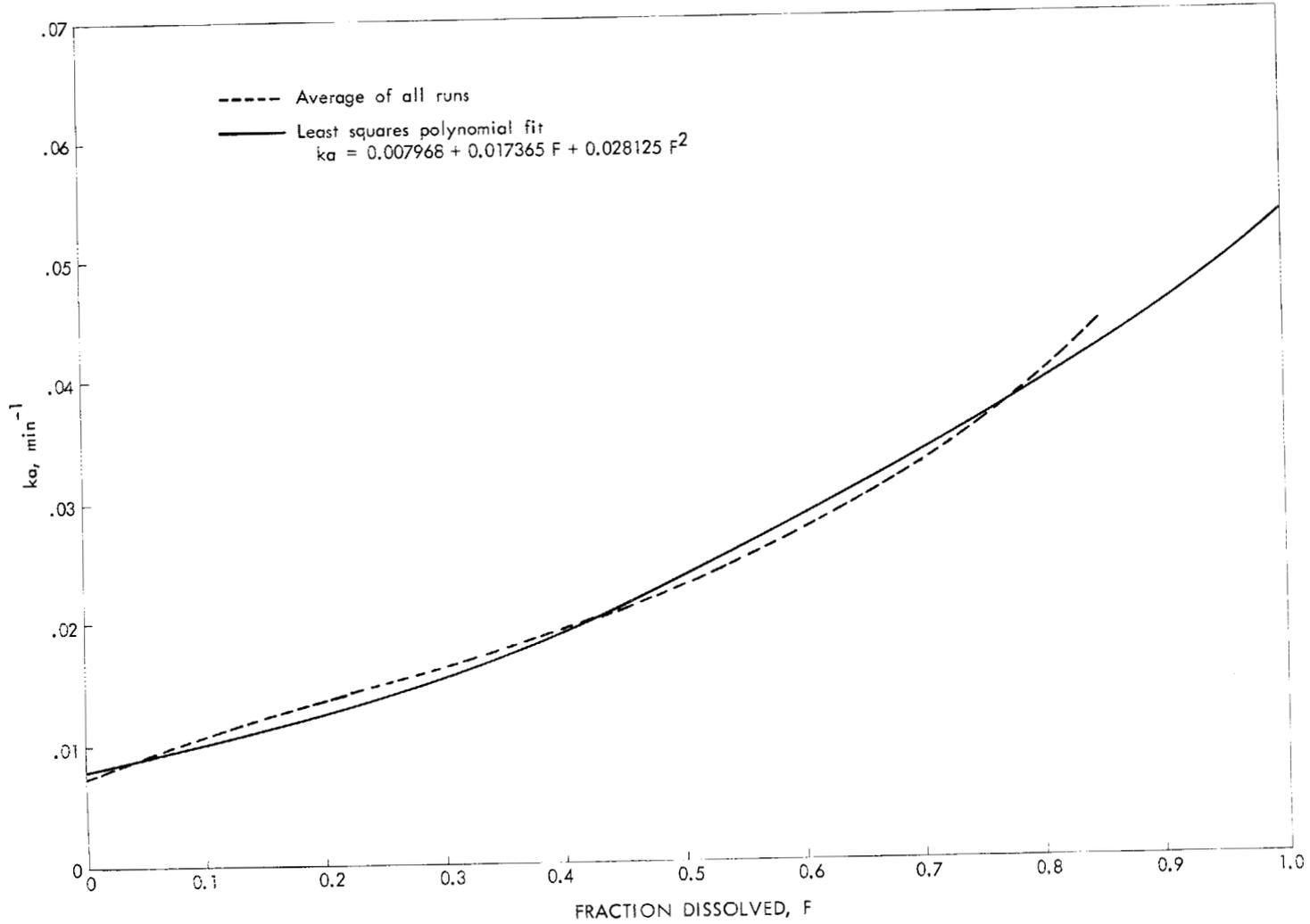


Fig. 22. Comparison of average k_a for all runs vs. fraction UO_2 dissolved with least squares polynomial fit.

5.0 APPLICATION OF k_a -vs- F RELATION

Having k_a as a function of F which applies approximately for eight runs made under varying conditions of flow rates and acid concentrations, an attempt was next made to use this relation with eqs. 4, 5, and 6 to compute relations of concentration and F vs time for the conditions of the experimental runs. Calculations were made on an analog computer, and the results were compared with the original experimental data.

Let the constants of eq. 14 be A , B , and C :

$$k_{a_n} = A + BF_n + CF_n^2 \quad (15)$$

The definition of F_n is

$$F_n = (m_o - m_n)/m_o = 1 - m_n/m_o \quad (16)$$

On eliminating r_n , m_n , and k_{a_n} between eqs. 4, 5, 6, 15, and 16, one obtains

$$\frac{dF_n}{dt} = A + \left\{ (B - A) + \left[(C - B) - CF_n \right] F_n \right\} F_n \quad (17)$$

and

$$- \frac{dC_n}{dt} = \frac{L}{V} (C_n - C_{n-1}) - \frac{m_o}{V} \frac{dF_n}{dt} \quad (18)$$

For scaling purposes, define X_n ,

$$X_n = C_n/C_R \quad (19)$$

where C_R is an arbitrarily selected reference concentration, preferably some value slightly greater than the maximum concentration in the problem. Now substitute eq. 19 in 18:

$$- \frac{dX_n}{dt} = \frac{L}{V} (X_n - X_{n-1}) - \frac{m_o}{C_R V} \frac{dF_n}{dt} \quad (20)$$

By using equations in which F_n and X_n are dependent variables whose magnitudes range between 0 and 1, magnitude scaling is automatically taken care of.

Observation of concentration profiles indicates that the concentration of one stage can be affected by concentrations in the two preceding stages, but that there is never any significant effect of earlier stages. Equations 15 and 20 apply to any stage, and these were set up three times so that three stages could be simulated simultaneously. The 221R Pace

Analog Computer in the Department of Chemical and Metallurgical Engineering at the University of Tennessee was used for this problem. Figure 23 shows the diagram for one stage. The other two were similar to this except that servo multipliers were used rather than the quarter-square electronic type shown in Fig. 23. The circuits for the three stages were connected through switches (Fig. 24).

Computer runs were made as follows:

1. Set potentiometers with appropriate values for run parameters.
2. For $n = 1$, open switches 00 and 01.
3. Set initial values for X_1 and F_1 at zero in stage n circuit.
4. Operate, plotting out values of X_1 and F_1 .
5. Hold operation at time t_0 and read X_1 and F_1 . These values are X_{11} and F_{11} , respectively.
6. Complete operation.
7. For $n = 2$, $n - 1 = 1$; close switch 01.
8. Set initial values of X_2 and F_2 at X_{11} and 0, respectively, in the n -stage circuit, and X_1 and F_1 at X_{11} and F_{11} in the $(n-1)$ -stage circuit.
9. Operate, plotting out X_2 and F_2 .
10. Hold operation at time t_0 and read X_2 , X_1 , F_2 , and F_1 . The values are X_{22} , X_{12} , F_{22} , and F_{12} , respectively.
11. Complete operation.
12. For $n = 3$, $n - 1 = 2$, $n - 2 = 1$; close switch 00.
13. Set initial values for X_3 and F_3 at X_{22} and 0, respectively, in the n -stage circuit, X_2 and F_2 at X_{22} and F_{22} in the $(n-1)$ -stage circuit, and X_1 and F_1 at X_{12} and F_{12} in the $(n-2)$ -stage circuit.
14. Operate, plotting out X_3 and F_3 . Hold operation at time t_0 and read X_3 , X_2 , F_3 , and F_2 . The values are X_{33} , X_{23} , F_{33} , and F_{23} , respectively.
15. Complete operation.
16. For $n = 4$, $n - 1 = 3$, $n - 2 = 2$, repeat procedure of step 12 and following.

Initial condition settings and switch settings are summarized in Table 3.

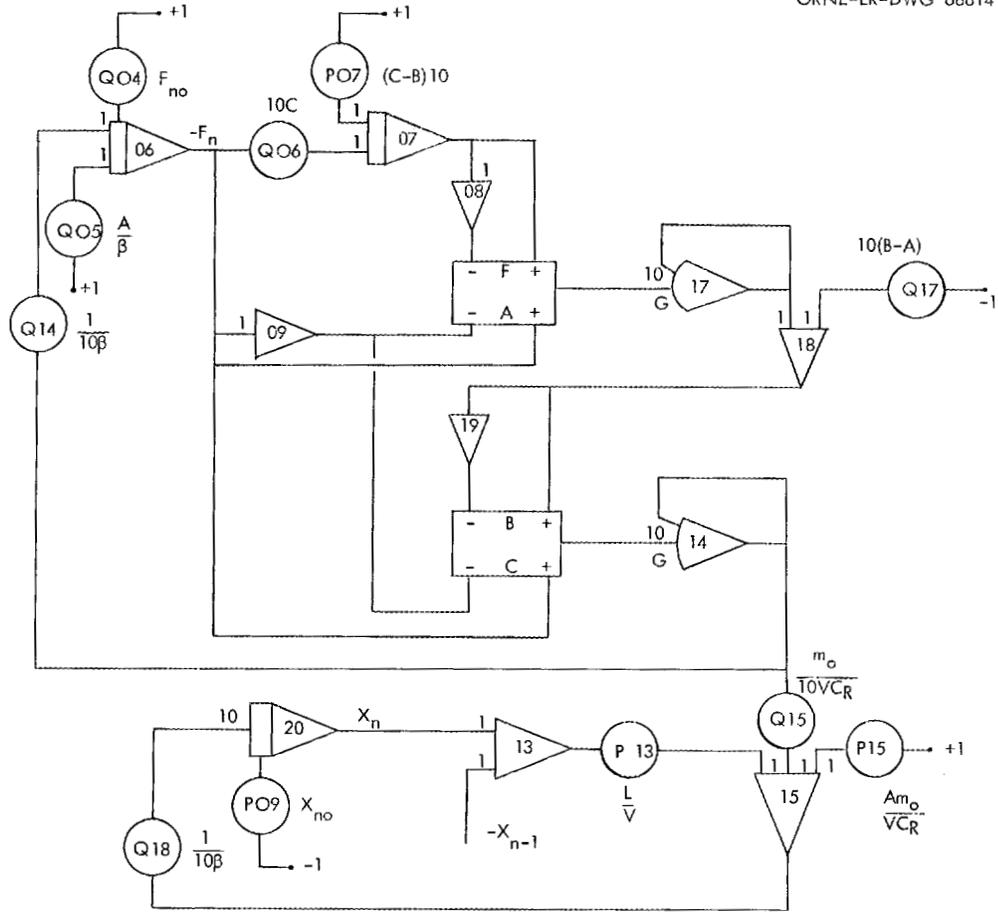


Fig. 23. Analog computer diagram, stage n.

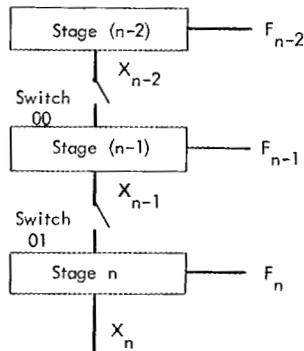


Fig. 24. Relation between analog computer circuits for three stages.

Table 3. Initial Condition Settings for Analog Computer Studies

No. of Stage (n)	Switch		Initial Conditions ^a					
	00	01	X_n	X_{n-1}	X_{n-2}	F_n	F_{n-1}	F_{n-2}
1	O	O	0	-	-	0	-	-
2	O	C	X_{11}	X_{11}	-	0	F_{11}	-
3	C	C	X_{22}	X_{22}	X_{12}	0	F_{22}	F_{12}
4	C	C	X_{33}	X_{33}	X_{23}	0	F_{33}	F_{23}

^aIn the double subscript notation, the first number refers to the stage number, and the second to the number of time units, t_0 , that have lapsed at the instant the appropriate value of X or F exists. For example, X_{22} is the relative concentration in the second stage at time $2t_0$, or at time t_0 after the second stage begins operation. (See Fig. 3 for a graphical representation of the X values.)

The results of analog computer runs for the cases of Table 1 are shown in the solid lines of Figs. 5 through 12. Agreement is generally fairly good between calculated and experimental concentration profiles. The first stage for each run usually shows poorest agreement. This is probably due to the fact that the agreement of k_a of eq. 14 (average for all stages of all runs) with k_a of the first stages is worse than with k_a 's of all the other stages. It should be remembered also k_a 's for the first stages are in greatest doubt because the experimental sampling intervals were large relative to the time required for the sharp concentration profile peaks to develop.

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