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A GENERALIZED COMPUTER PROGRAM
FOR FLOWSHEET CALCULATION
AND PROCESS DATA REDUCTION

by

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SUMMARY

A generalized computer program, PACER-65, has been developed and utilized for flowsheet calculations and process-data reduction. PACER-65 is an executive program in which material- and energy-balance equations, conversion factors, etc., for each processing step are described by separate subroutines. The program plans the sequence of the calculations and calls the subroutines in the order required to determine all desired properties of the process streams. The effects of changes in the process flowsheet or variation of processing conditions are readily evaluated. The PACER-65 method has also been adapted for process-data reduction. In this case, the subroutines incorporate calibration data for flow-metering instruments, etc., as well as equations required to perform the various calculations.

Examples of these applications to fluid-bed volatility processes are presented.

I. INTRODUCTION

A computer program, PACER-65, has been developed and utilized for flowsheet calculations and process-data reduction in the Chemical Engineering Division of Argonne National Laboratory. This report describes the program and presents examples of its application.

In broad terms, PACER-65 is an executive program for flowsheet calculations. Each unit, vessel, meter, processing operation, etc., in the

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overall flowsheet is represented by a separate subroutine, which is completely removable and interchangeable. The subroutines generally contain material- and/or energy-balance equations, calibration data, conversion factors, etc. The PACER-65 executive program calls the various subroutines in the order required to complete an overall flowsheet calculation.

The advantages offered by PACER-65 are:

(1) The process designer is relieved, as much as possible, of the tedious aspects of flowsheet studies. This provides him with more time to generate new ideas for flowsheet improvement and with rapid access to the results of any suggested flowsheet changes. For example, removal or addition of a recycle stream to a flowsheet may be as simple as altering a few numbers on a data card or, at most, as "difficult" as providing one or two subroutines to describe the recycle conditions. Variation of process conditions (such as a vessel temperature) or processing rates can be completely investigated by simple changes in the data. Detailed knowledge of the computer program is not required.

(2) PACER-65 is constructed in a manner similar to the actual process flowsheet. Thus, each process vessel is represented by a separate equipment subroutine, and the PACER-65 executive program is provided with a simple numerical code telling how the process equipment vessels are connected in the flowsheet. The process-equipment subroutines are mutually compatible so that once a subroutine describing, for example, the material balances in a hydrochlorinator has been written, this subroutine may be used to represent hydrochlorination in any PACER-65 flowsheet for which design calculations are to be performed. This materially simplifies use of the computer for flowsheet calculations, because the amount of programming required to investigate new or alternative flowsheets, or flowsheet modifications, is minimized.

(3) The executive portion of PACER-65 is almost fully automatic. If desired by the user, it will automatically set up and execute an iterative pattern and convergence tests to carry out any trial-and-error calculations, such as might be required by the presence of recycle. Alternatively, the user can specify to the executive-program information such as which of the unknown stream flow rates are to be assumed as known, what should be the value of the initial assumption, or what convergence test should be applied. In any case, the executive program plans the entire order of the calculations, and proceeds from vessel to vessel to calculate flow rates, velocities, temperatures, pressures, and all desired properties of the process streams. This automation contributes significantly to the reduction in the programming time required for computerizing flowsheet calculations.

The PACER concept was originally presented by H. A. Mosler.¹ This reference should be consulted for further details.

II. BASIC DESCRIPTION OF EXECUTIVE PROGRAM FOR PACER-65

The function of the executive program is illustrated by an example involving flowsheet calculations for a process in which uranium-alloy fuel elements are reacted with hydrogen chloride to separate the cladding and alloying material from the uranium. For simplicity in the subsequent sections of this report, this hydrochlorination step is referred to as a decladding operation. Previous development studies²⁻⁴ with uranium-aluminum and uranium-zirconium alloy fuels have established suitable reaction conditions for this decladding operation. The process flowsheet is given in Fig. 1.

Fig. 1. Process Flowsheet for Decladding by Hydrochlorination

A. Description of Process Flowsheet for Hydrochlorination Example

For this example, only gross calculations are performed. The presence of uranium and minor components in the fuel elements, the partial pressures of water at room temperature over aqueous HCl solutions, and similar refinements are omitted for clarity.

The cladding and alloying element, zirconium or aluminum, is charged to the hydrochlorinator at a given rate. The hydrochlorinator has a given efficiency of utilization of HCl in the reaction

or

This efficiency is determined by the reaction temperature and HCl feed rate. The volume percent of hydrogen in the H_2 -HCl recycle gas feed is specified. Gaseous reaction products from the hydrochlorinator are treated with steam (containing recovered HCl) in the pyrohydrolyzer to convert the cladding element to oxide*

The efficiency of utilization of the steam is also specified. The gaseous products of the pyrohydrolyzer are condensed at ambient conditions, at which the solubility of HCl is 42% by weight in water. The stream of non-condensed HCl and H_2 from the condenser is divided into a hydrochlorinator recycle stream and a stream which is to be treated with water in a scrubbing tower for further HCl recovery. The scrubber is also operated at ambient conditions to give an HCl-rich liquid effluent which is combined in a boiler with the condensate from the condenser. The vaporized boiler effluent serves as the feed gas for the pyrohydrolyzer. Undissolved gaseous HCl and H_2 from the scrubber are sent to disposal. Any makeup HCl required as a result of this disposal is combined with the recycle HCl- H_2 stream to form the reactor feed gas. Note that the "Divider" and "Combiner" vessels shown on the flowsheet are included only for analogy with the information flowsheet, shown in Fig. 2. There would likely be no corresponding vessels in the process flowsheet; the division and combination could occur in a simple tee.

Fig. 2. Information Flowsheet for Decladding by Hydrochlorination

B. Information Flowsheet

From the previous description it follows that the overall stoichiometry has been approximated by

Since no water is assumed to leave the process flowsheet, the water fed to the scrubbing tower must be precisely at the stoichiometric rate required to oxidize the zirconium or aluminum feed. With reference to the information flowsheet of Fig. 2, this fact is indicated by the "flow" of an H_2O "stream" (stream 13) from the hydrochlorinator (vessel 1) to the scrubber (vessel 5). Thus, the information flowsheet describes the flow of information for process calculations.

The following simple rules govern the construction of an information flowsheet:

- (1) Each process vessel is represented by a numbered box.
- (2) A stream is designated as an input to a process vessel (or box) if the information in that stream (e.g., flow rate of some component or components) is to be used in performing material and/or energy balances on that process vessel.
- (3) A stream is designated as an output of a process vessel if the information in that stream is acquired as a result of performing the material and/or energy balances on that process vessel.
- (4) A single process stream may be represented as several information streams if parts of the information in that stream are to be used as information in different process vessels. Alternatively, several process streams may be collapsed into one information stream if the information flow so warrants.
- (5) It is expressly guaranteed by the information flow diagram that, when all input information streams to a given box are known, all output streams from that box can be calculated and therefore become known information streams. The calculations are performed by a program called the equipment subroutine, which represents the process vessel.
- (6) When convenient, boxes may be used to represent imaginary process vessels, on both the process and information flowsheets. This is usually done to represent combination of two or more process streams,

or division of a single process stream into several process streams, as in a recycle flowsheet. In general, wherever calculations of material and/or energy balance are to be performed, there must be a box, i.e., a box implies calculations, and vice versa.

These rules are explained through use of the information flowsheet of Fig. 2, which represents the process flowsheet of Fig. 1.

Consider the vessels in the order numbered. Box 1 represents the hydrochlorinator, and input stream 1 represents the rate at which the cladding and alloying element (assumed for this explanation to be zirconium) is to be volatilized. Stream 1 is assumed to be known (alternatively, it may be taken at some arbitrary value since it represents only a scale factor). Since the efficiency of utilization of HCl in the hydrochlorinator and the composition of the feed gas (e.g., percent hydrogen) are specified parameters, the flow rates of H_2 (stream 12) and HCl (stream 15) in the gas feed may be calculated by simple material balance. Correspondingly, the required rate of input of water (stream 13) to the process (in the scrubber influent) can also be calculated from the specified zirconium rate in stream 1. The rates of production of $ZrCl_4$, H_2 , and HCl can be calculated and are collapsed to information stream 2, shown as an output of box 1 and as an input to box 2, the pyrohydrolyzer. It may be seen that stream 2 corresponds exactly to a process stream, while the other outputs of box 1 differ in some aspect from any streams on the process flow diagram. Thus, since the HCl feed rate is calculated by box 1, this stream appears as an output of this box, rather than as an input stream as it does on the process flowsheet; a similar statement applies to the H_2 feed rate. Also, while the HCl and H_2 form a single process stream, they are separated into two information streams. The reason for this is that the H_2 flow rate will later be used to determine the recycle split, in box 4, while the HCl flow rate will be used to calculate the required flow rate of makeup HCl, in box 7. Hence, these are shown as input information streams to their respective boxes.

Next, consider the pyrohydrolyzer, represented by box 2. Knowledge of the $ZrCl_4$ flow rate from box 1, the HCl flow rate (stream 9) from the boiler (box 6), and the efficiency of utilization of steam guarantees that the necessary H_2O rate from the boiler (stream 10), the rate of production of ZrO_2 (stream 11), and the effluent rates of H_2O , HCl, and H_2 (stream 3) can be calculated. Note that output streams 3 and 11 correspond to process streams, while input stream 9 and output stream 10 do not; these latter two are parts of a process stream, and go in different directions because of the algorithm used.

The situation in box 3 corresponds exactly to the process flowsheet. No further discussion is required.

Box 4 represents the division of the uncondensed H_2 -HCl stream into a reactor recycle stream and an HCl recovery stream. The split is made on the basis of the H_2 feed rate required for the hydrochlorinator reactor, box 1. This rate and the rate of stream 4 are the inputs to box 4. The outputs of box 4 are the rates of the H_2 -HCl streams going to reactor recycle (stream 14) and to the scrubber (box 5) for further HCl recovery (stream 5).

The information inputs to box 5 are the water feed rate and the HCl- H_2 feed rate. The calculations performed by box 5 involve use of the solubility of HCl in water at the scrubber conditions to determine the amount of HCl absorbed into stream 7, the boiler feed. Any unabsorbed HCl is combined with the H_2 to form information stream 6, corresponding to the process gas disposal stream.

The boiler (box 6) simply adds the HCl flows in input streams 7 and 8 to determine output stream 9, the HCl feed rate to the pyrohydrolyzer (box 2). This represents the total HCl recovered in the condenser and scrubber.

Box 7 is a hypothetical combiner, and compares the HCl in recycle stream 14 with the HCl required in the reactor feed stream 15, to compute the HCl makeup requirement, stream 16. Obviously this must be equal to the HCl lost in stream 6, and this provides an overall check on the computations.

All boxes used are now "standard" equipment subroutines. For example, box 1 may be used in any flowsheet to represent hydrochlorination where the feed gas composition and reaction efficiency are specified. This is true because the box merely performs a specified set of calculations on the input streams to yield values in the output streams.

C. The Process Matrix

The PACER-65 executive routine is provided with access to a complete library of these equipment subroutines. It remains only to indicate to PACER-65 how the various information streams flow from one piece of equipment to the other, i.e., to describe the information flow diagram. This is done by providing as input data the Process Matrix (PM).

The first column of the PM gives the box numbers (in arbitrary order). In the row next to each box number follows a list of stream numbers for that box. Input stream numbers appear first, with positive signs, and output stream numbers next with negative signs. Thus, for the information flowsheet of Fig. 2, the PM appears as follows:

1	1	-2	-12	-13	-15
2	2	9	-3	-10	-11
3	3	-4	-8		
4	4	12	-5	-14	
5	5	13	-6	-7	
6	7	8	-9		
7	14	15	-16		

D. The Basic Algorithm

The PACER-65 executive routine begins by scanning the PM. When it finds a row (corresponding to a particular piece of equipment or "box") for which all input (positive) stream numbers have known flow rates, i.e., are known streams, it recognizes that it can calculate the flow rates of all output streams whose numbers appear (with negative signs) in that row. The equipment subroutine is called, the calculated flow rates are stored, and the output streams are now marked as known everywhere they appear in the PM. For example, in the PM just described, PACER would recognize that, since stream 1 is a known input stream, streams 2, 12, 13, and 15 may be calculated by calling the hydrochlorinator subroutine. After the calculations are completed, it marks these streams as known, and continues to scan the PM to find another row for which all input streams are known. In the present example, none are available.

When a condition of no calculable rows in the PM exists, a trial-and-error recycle calculation (or possibly a programming error) is sought. PACER proceeds as follows: It tries to find one stream number such that, if that stream were assumed to be known, the calculations could continue and eventually reach a point where the stream previously assumed to be known, could be calculated directly, thus setting up an iterative procedure. If desired, the user can point out the existence of such a stream, and a good first assumption for the flow rate. If no such first assumption is indicated, PACER will "guess" zero. In the preceding example, it is indicated in the data that stream 9 can be so used, and a first assumption is not indicated because zero is satisfactory. The calculations then proceed in the following manner, as set up by the PACER executive program:

<u>Using Streams</u>	<u>In Row</u>	<u>Calculate Streams</u>	<u>By Calling Equipment Subroutine for</u>
2,9	2	3,10,11	Pyrohydrolyzer
3	3	4,8	Condenser
4,12	4	5,14	Divider
5,13	5	6,7	Scrubber
7,8	6	9	Boiler (combiner)

TABLE 1. Flowsheet Calculations for Reprocessing Enriched Uranium-Zirconium Alloy Fuel

Case I				Case II 2				Case III			
FUEL RATE = 10.00 KG/HR				FUEL RATE = 10.00 KG/HR				FUEL RATE = 10.00 KG/HR			
EFFICIENCY OF HYDROCHLORINATOR = 5.00				EFFICIENCY OF HYDROCHLORINATOR = 5.00				EFFICIENCY OF HYDROCHLORINATOR = 80.00			
PERCENT HYDROGEN TO HYDROCHLORINATOR = 10.00				PERCENT HYDROGEN TO HYDROCHLORINATOR = 80.00				PERCENT HYDROGEN TO HYDROCHLORINATOR = 80.00			
EFFICIENCY OF PYROHYDROLYSER = 33.30				EFFICIENCY OF PYROHYDROLYSER = 33.30				EFFICIENCY OF PYROHYDROLYSER = 33.30			
PERCENT WATER FROM CONDENSER = 58.00				PERCENT WATER FROM CONDENSER = 58.00				PERCENT WATER FROM CONDENSER = 58.00			
	KG/HR	V/O	W/O		KG/HR	V/O	W/O		KG/HR	V/O	W/O
TO HYDROCHLORINATOR				TO HYDROCHLORINATOR				TO HYDROCHLORINATOR			
HCL	319.7983	0.900		HCL	319.7983	0.200		HCL	19.9874	0.200	
H2	1.9645	0.100		H2	70.7213	0.800		H2	4.4201	0.800	
FROM HYDROCHLORINATOR				FROM HYDROCHLORINATOR				FROM HYDROCHLORINATOR			
FCL	25.5426	0.011		FCL	25.5426	0.003		FCL	25.5426	0.042	
HCL	303.8084	0.865		HCL	303.8084	0.190		HCL	3.9975	0.042	
H2	2.4065	0.124		H2	71.1633	0.807		H2	4.8621	0.917	
GAS FROM PYROHYDROLYSER				GAS FROM PYROHYDROLYSER				GAS FROM PYROHYDROLYSER			
H2O	7.9119	0.041		H2O	7.9119	0.010		H2O	7.9119	0.122	
HCL	328.3879	0.847		HCL	327.5263	0.201		HCL	27.7154	0.210	
H2	2.4065	0.112		H2	71.1633	0.789		H2	4.8621	0.668	
OXIDE FROM PYROHYDROLYSER				OXIDE FROM PYROHYDROLYSER				OXIDE FROM PYROHYDROLYSER			
FO	13.5080		1.000	FO	13.5080		1.000	FO	13.5080		1.000
GAS FROM CONDENSER				GAS FROM CONDENSER				GAS FROM CONDENSER			
HCL	322.6586	0.881		HCL	321.7970	0.200		HCL	21.9861	0.200	
H2	2.4065	0.119		H2	71.1633	0.800		H2	4.8621	0.800	
GAS TO SCRUBBER				GAS TO SCRUBBER				GAS TO SCRUBBER			
HCL	59.2638	0.881		HCL	1.9987	0.200		HCL	1.9987	0.200	
H2	0.4420	0.119		H2	0.4420	0.800		H2	0.4420	0.800	
FEED WATER				FEED WATER				FEED WATER			
H2O	3.9500		1.000	H2O	3.9500		1.000	H2O	3.9500		1.000
TO DISPOSAL				TO DISPOSAL				TO DISPOSAL			
HCL	56.4035	0.876		HCL	0.0000	0.000		HCL	0.0000	0.000	
H2	0.4420	0.124		H2	0.4420	1.000		H2	0.4420	1.000	
LIQUID FROM SCRUBBER				LIQUID FROM SCRUBBER				LIQUID FROM SCRUBBER			
HCL	2.8604		0.420	HCL	1.9987		0.336	HCL	1.9987		0.336
H2O	3.9500		0.580	H2O	3.9500		0.664	H2O	3.9500		0.664
LIQUID FROM CONDENSER				LIQUID FROM CONDENSER				LIQUID FROM CONDENSER			
HCL	5.7293		0.420	HCL	5.7293		0.420	HCL	5.7293		0.420
H2O	7.9119		0.580	H2O	7.9119		0.580	H2O	7.9119		0.580
FROM BOILER				FROM BOILER				FROM BOILER			
HCL	8.5896	0.263		HCL	7.7280	0.244		HCL	7.7280	0.244	
H2O	11.8619	0.737		H2O	11.8619	0.756		H2O	11.8619	0.756	
RECYCLE				RECYCLE				RECYCLE			
HCL	263.3948	0.881		HCL	319.7983	0.200		HCL	19.9873	0.200	
H2	1.9645	0.119		H2	70.7213	0.800		H2	4.4201	0.800	
MAKE-UP HCL GAS				MAKE-UP HCL GAS				MAKE-UP HCL GAS			
HCL	56.4035	1.000		HCL	0.0000	0.000		HCL	0.0000	0.000	

Note: FCI and FO are used to designate the chloride and oxide of the cladding element, respectively.

The resulting value of stream 9 provides a check on the initial assumption, and the process is iterated until assumed and calculated values agree.

At the completion of this iteration, only stream 16 remains to be calculated, and this is possible because streams 14 and 15 are known.

It should be emphasized that any number of different information flow diagrams may be used to describe a given process flowsheet. In specifying a particular information flowsheet and PM, such as the one described above, the user is really planning his method of calculating the flowsheet, and communicating this information to PACER.

If PACER is unable to find a single stream which may be assumed known and thereby set up an iterative procedure, it will seek a combination of two streams which will yield a suitable iteration; failing this, it will search for a combination of three streams. If neither a second- nor third-order recycle iteration can be set up, PACER quits and indicates a programming error. At present, capability for a third-order iteration appears adequate to handle the great majority of process situations. However, if required, the executive program may be expanded to allow calculations of higher order.

E. Flowsheet Alteration

It is easy to make alterations in the flowsheet when PACER is used. For example, to investigate the possibility of elimination of the scrubber, the user has only to supply the following PM in place of the previous one:

1	1	-2	-12	-13	-15
2	2	9	-3	-10	-11
3	3	-4	-8		
4	4	12	-5	-14	
6	7	8	-9		
7	14	15	-16		

Stream 7 would not be indicated in the data deck as a known stream, with flow rate zero.

F. Results of Example

Results which may be obtained from PACER-65 are illustrated by Cases I, II, and III in Table 1, which are reproductions of a portion of the output for the zirconium-hydrochlorination example. The three cases respond to the following variations in process conditions:

Case	Hydrochlorinator Efficiency (%)	Hydrogen in Hydrochlorinator Feed (v/o)
I	5	10
II	5	80
III	80	80

Comparison of the output data for Cases I and II shows that increasing the percent of hydrogen in the reactor feed removes the necessity for HCl makeup (except for small quantities indicated by practical considerations not included in these illustrative calculations). Cases II and III give an assessment of the reduction in gas flow rates which can be achieved by operating at higher efficiencies of utilization of HCl, corresponding to higher reactor temperatures. The calculations for each table require approximately one second of CDC-3600 time, and therefore any number of process conditions may be investigated at negligible cost.

III. DATA-REDUCTION CALCULATIONS WITH PACER-65

Although the PACER-65 method is primarily designed for flow-sheet calculations, it is easily adapted to process-data reduction. For the present discussion, data reduction is defined as conversion of raw process data, such as orifice pressure drop or millivolt readings, to quantities such as flowrate, temperature, and efficiencies of reactions. The calculations necessary for this data reduction are systematized by application of PACER-65 so that changes in the process flowsheet or instrument calibrations are easily incorporated into the program.

Basically, the only difference between applications involving flow-sheet calculation and those involving data reduction is which information streams are considered as inputs to a given unit, and which are considered outputs. For example, the concentration of a product in a reactor effluent would likely be output information from the reactor in flowsheet calculations; this same quantity would be input information for data reduction when the concentration is monitored during the process run.

A great number of the units (or boxes) in the data-reduction application will be representations of calibration curves. For example, a pressure-drop reading will be input information to a box which then "computes" a flowrate by interpolation⁵ in the calibration data provided as parameters for the box.

The potential savings in manpower which can be achieved by using PACER-65 to perform these tedious, repetitive calculations make further

study of this application desirable. Use of automatic data-logging equipment for the transfer of data from process instrumentation to the computer is recommended. Where automatic data-plotting facilities are associated with a computer, graphical output of data calculated by PACER-65 may also be obtained.

The subsequent sections contain descriptions of applications of PACER-65 to reduction and reporting of data obtained from three different processing units.

A. Application to Pilot-plant Fluorination of UO_2 Pellets

PACER-65 has been used to calculate experimental results from the data obtained in fluorination pilot-plant runs. Currently, variables in the fluorination of nuclear reactor-grade, uranium dioxide pellets are being studied in the pilot plant. Details of the equipment used in the investigation have been described previously by Vogel *et al.*⁶

A schematic equipment flowsheet is shown in Fig. 3. The equipment includes a fluid-bed fluorinator with connected off-gas filters, a secondary off-gas filter, two hexafluoride desublimation cold traps, a gas-circulating pump, a fluorine analyzer, and chemical traps for removing fluorine and hexafluorides from the process off-gas stream.

Fig. 3. Fluorination Process Equipment--Pilot-plant Fluorinator (Symbols--See Table 2)

The cylindrical uranium dioxide pellets are charged into a fluidized bed of chemically inert, sintered alumina to form two zones--a lower, fluidized-packed bed of pellets and an upper, fluidized alumina bed. Oxygen, diluted with nitrogen, is passed through the oxide pellets, forming U_3O_8 , which spalls from the pellet surface and is carried by the gas stream to the upper zone. Here the U_3O_8 reacts with fluorine, added through an inlet located above the pellets, to form uranium hexafluoride (UF_6).⁷ The reactions are:

The overall reaction is

The upper zone temperature is held at 450°C. In the lower zone, a temperature gradient, with 450°C at the top of the pellet bed and generally 350°C at the bottom, is used to promote the reaction rate and thus fines formation in the upper part of the pellet bed, where the fines can be transported easily. The UF_6 product, fluorine, oxygen, and diluent nitrogen leave the fluorinator and filters and pass into two cold traps, in which the UF_6 is desublimed by cooling the gas stream to approximately -60°C.

The variables pertinent to the computer calculation program are shown in Fig. 3 and listed in Table 2. Flows other than those listed are also metered as a check on the listed flow rates. Typical calibration data used to calculate flow rates from pressure-drop measurements across an orifice plate are shown in Table 3; these data are printed out by the computer as a permanent record. The calculated quantities and the equations for calculating them are given in Table 4. Exit gas from the cold traps is analyzed for fluorine content to check the calculated fluorine efficiency. A portion of a typical computer output sheet is presented in Table 5. Some calculated results were plotted with the use of a Calcomp 580 plotter, and typical examples of these plots are shown in Fig. 4.

B. Application to Bench-scale Fluorination of UO_2 - PuO_2 -Fission Product Pellets

Development studies are in progress using a 2-in.-diameter fluid-bed reactor to determine optimum fluorination conditions for UO_2 - PuO_2 -fission product oxide pellets. Two fluorination agents are being evaluated:

fluorine and bromine pentafluoride (BrF_5). Fluorination with dilute fluorine is carried out by a simultaneous oxidation-fluorination technique,⁷ as described in the previous section. During this process step, most of the uranium and approximately half of the plutonium are converted to the volatile hexafluorides. Residual plutonium and final traces of uranium are volatilized from the fluidized alumina bed by reaction with 90 v/o fluorine.⁸ In the second process, fluorination with bromine pentafluoride is carried out after the pellets are reacted with oxygen in a separate step. During fluorination with bromine pentafluoride, only the uranium is volatilized as hexafluoride product, leaving a residue of plutonium compounds which are subsequently fluorinated to plutonium hexafluoride by reaction with fluorine. The use of bromine pentafluoride as a selective fluorinating agent enables a separation of the uranium from the plutonium to be achieved in the fluid-bed fluorinator.

TABLE 2. Process Variables Pertinent to Computer Calculations--
Pilot-plant Fluorinator

Symbol	Variable
F_{tb}	Total gas flow rate into bottom inlet of the fluorinator,* cfm
P_{tb}	Pressure at metering orifice, total bottom flow rate, psig
F_{ts}	Total gas flow rate into side inlet of the fluorinator,* cfm
P_{ts}	Pressure at metering orifice, total side flow rate, psig
F_{F_2}	Fluorine gas flow rate into fluorinator,* cfm
P_{F_2}	Pressure at metering orifice, fluorine, psig
F_{O_2}	Oxygen gas flow rate into fluorinator,* cfm
P_{O_2}	Pressure at metering orifice, oxygen, psig
P_r	Pressure in fluorinator, psig
T_1	Temperature in pellet bed zone of fluorinator, °C
T_u	Temperature in fluidized bed zone of fluorinator, °C
$\Delta\theta$	Data reading time interval, min

*The differential pressure across the orifice is recorded. This value (actually the chart reading is used) and the pressure at the orifice are used as input for an equipment subroutine⁵ in which the flow rate is determined.

TABLE 3. Typical Flowrate Calibration Data--
Pilot-plant Fluorinator

FRC-38 (TOTAL BOTTOM FLOW)					P_{tb}
PRES (PSIG)	0.0	5.0	10.0	20.0	
IN. H ₂ O / SCFM					
0.00	0.00	0.00	0.00	0.00	} F_{tb}
1.00	0.63	0.73	0.81	0.96	
2.00	0.92	1.07	1.20	1.42	
3.00	1.15	1.33	1.50	1.77	
4.00	1.36	1.58	1.77	2.10	
5.00	1.55	1.80	2.02	2.39	

TABLE 4. Formulas Used in Computer Calculations--
Pilot-plant Fluorinator

$$W_{UF_6}, \text{ collection rate, g/min} = \left[\frac{\Delta \text{ millivolts}^*}{\Delta \theta} \right] \left[\frac{\text{calibration}}{\text{factor}} \left(\frac{\text{g}}{\text{millivolts}} \right) \right]$$

$$w_{UF_6}, \text{ collection rate, lb/hr} = \left[W_{UF_6} \right] \left[\frac{1 \text{ lb}}{453.6 \text{ g}} \right] \left[\frac{60 \text{ min}}{1 \text{ hr}} \right]$$

$$V_{UF_6}, \text{ collection rate, scfm} = \left[W_{UF_6} \right] \left[\frac{1 \text{ lb}}{453.6 \text{ g}} \right] \left[\frac{359 \text{ ft}^3}{352 \text{ lb}} \right]$$

$$V_1, \text{ superficial gas velocity, lower or pellet zone, ft/sec} = \left[F_{tb} \right] \left[\frac{T_1 + 273}{273} \right]$$

$$\left[\frac{14.7}{P_r + 14.7} \right] \left[\frac{1 \text{ min}}{60 \text{ sec}} \right] \left[\frac{1}{0.0513 \text{ ft}^2} \right]$$

Note: 0.0513 ft^2 = cross-sectional area of 3-in.-diameter reactor.

$$V_u, \text{ superficial gas velocity, upper or fluidized bed zone, ft/sec} =$$

$$\left[F_{tb} + T_{ts} - \frac{\text{oxygen reacted}}{\text{in pellet bed}} \right] \left[\frac{T_u + 273}{273} \right] \left[\frac{14.7}{14.7 + P_r} \right] \left[\frac{1 \text{ min}}{60 \text{ sec}} \right] \left[\frac{1}{0.0513 \text{ ft}^2} \right]$$

$$\text{Note: Oxygen reacted in pellet bed, ** scfm} = \left[V_{UF_6} \right] \left[\frac{1 \text{ mol O}_2}{3 \text{ mol UF}_6} \right]$$

$$O_2 \text{ utilization, **\%} = \frac{1}{3} \left[V_{UF} \right] \left[\frac{1}{F_{O_2}} \right] [100]$$

$$F_2 \text{ utilization, **\%} = 3 \left[V_{UF_6} \right] \left[\frac{1}{F_{F_2}} \right] [100]$$

$$\text{Fluorine in process off-gas, **\%} = \frac{F_{F_2} - 3[V_{UF_6}]}{F_{ts} + F_{tb} - 2[V_{UF_6}]} [100]$$

$$UF_6 \text{ production rate per reactor area, lb/(hr)(ft}^2) = \frac{w_{UF_6}}{0.0513 \text{ ft}^2}$$

Cumulative volume of fluorine fed to the reactor at the end of time period $n = i$,

$$\text{ft}^3 = \sum_{n=0}^{n=i} [F_{F_2}]_i [\Delta \theta]_i$$

TABLE 4. (Contd.)

Cumulative volume of oxygen fed to the reactor at the end of time period $n = i$,

$$ft^3 = \sum_{n=0}^{n=i} [F_{O_2}]_i [\Delta\theta]_i$$

Cumulative weight of UF_6 collected in cold trap at the end of time period $n = i$,

$$g = \sum_{n=0}^{n=i} [W_{UF_6}]_i [\Delta\theta]_i$$

Percent of total UF_6 collected at the end of time period $n = i$,

$$\% = \frac{\sum_{n=0}^{n=i} [W_{UF_6}]_i [\Delta\theta]_i}{\sum_{n=0}^{n=j} [W_{UF_6}]_i [\Delta\theta]_i} [100]$$

where $n = j =$ last time period.

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*The weighing scales for the UF_6 cold traps generate a millivolt signal which is recorded.

**These equations neglect the effect of possible accumulation of U_3O_8 and UO_2F_2 fines in the fluid bed reactor.

TABLE 5. Computer Output Data Sheet--Pilot-plant Fluorinator

TIME	TEMPERATURE		PRES	INPUT	FLOW	CUM.	F2 IN	VELOCITY		PERCENT		RATE OF UF6		CUM.	UF6	PERCENT
	LOWER	UPPER	PSIG	RATES	(SCFM)	F2	OFF GAS	(FT/SEC)		UTILIZATION		VOL.	WT.	UF6	LB/HR/	TOTAL
	(C)	(C)		F2	O2	(SCF)	(O/O)	UPPER	LOWER	O2	F2	SCFH	LB/WR	(GM)	SO. FT.	UF6
0	420	440	6.1	0.000	0.000	0.0	0.0	1.108	0.786	0.0	0.0	0.000	0.000	0.0	0.0	0.0
10	420	440	6.1	0.153	0.388	1.5	7.6	1.108	0.786	0.4	9.1	0.278	0.272	20.6	5.3	0.2
20	420	440	6.1	0.172	0.391	3.2	8.9	1.108	0.786	0.2	4.2	0.145	0.142	31.3	2.8	0.3
30	465	435	4.6	0.208	0.384	5.3	6.4	1.178	0.898	2.7	44.9	1.867	1.830	169.8	35.7	1.5
40	465	435	4.6	0.096	0.037	6.3	0.5	1.179	0.898	24.1	90.0	1.722	1.689	297.6	32.9	2.7
50	465	435	4.6	0.216	0.000	8.4	4.1	1.174	0.898	0.0	66.6	2.878	2.822	511.2	55.0	4.6
100	465	420	4.6	0.194	0.000	10.4	12.7	0.834	0.606	0.0	14.3	0.556	0.545	552.4	10.6	4.9
110	465	420	4.6	0.068	0.071	11.1	-0.9	0.831	0.606	12.4	117.2	1.589	1.558	670.3	30.4	6.0
120	465	420	4.6	0.178	0.000	12.9	9.8	0.833	0.606	0.0	29.0	1.033	1.013	746.9	19.8	6.7
130	410	442	5.8	0.115	0.054	14.0	4.6	0.999	0.664	0.3	35.3	0.811	0.795	807.1	15.5	7.2
140	410	442	5.8	0.209	0.225	16.1	10.8	1.000	0.664	1.7	16.2	0.678	0.665	857.4	13.0	7.7
150	410	442	5.8	0.218	0.107	18.3	2.9	0.990	0.664	18.0	80.0	3.489	3.421	1116.3	66.7	10.0
200	405	440	4.1	0.230	0.065	20.6	-0.4	1.144	0.743	40.5	102.6	4.711	4.620	1465.8	90.1	13.1
210	405	440	4.1	0.234	0.000	22.9	0.0	1.144	0.743	0.0	99.9	4.678	4.587	1812.9	89.4	16.2
220	405	440	4.1	0.290	0.000	25.8	-2.0	1.137	0.743	0.0	110.8	6.434	6.308	2290.3	123.0	20.5
230	390	465	6.8	0.328	0.000	29.1	-6.3	1.017	0.645	0.0	128.0	8.412	8.248	2914.3	160.8	26.0
240	390	465	6.8	0.309	0.104	32.2	0.5	1.025	0.645	32.0	97.3	6.012	5.894	3360.3	114.9	30.0
250	390	465	6.8	0.181	0.104	34.0	3.7	1.037	0.645	12.7	65.8	2.389	2.343	3537.6	45.7	31.6
300	400	440	6.4	0.042	0.104	34.4	-0.3	1.032	0.748	5.1	114.1	0.956	0.937	3608.5	18.3	32.2
310	400	440	6.4	0.053	0.107	35.0	2.3	1.034	0.748	1.4	26.1	0.278	0.272	3629.1	5.3	32.4
320	400	440	6.4	0.196	0.107	36.9	9.1	1.032	0.748	4.0	19.6	0.767	0.752	3686.0	14.7	32.9
330	460	457	6.7	0.251	0.107	39.4	12.1	1.160	0.809	1.8	7.1	0.356	0.349	3712.4	6.8	33.2
340	460	457	6.7	0.250	0.107	41.9	9.7	1.157	0.809	4.8	26.5	1.322	1.297	3810.5	25.3	34.1
350	460	457	6.7	0.241	0.107	44.3	3.6	1.150	0.809	14.0	72.5	3.489	3.421	4069.4	66.7	36.4
400	445	445	7.2	0.242	0.107	46.7	2.0	1.090	0.776	21.4	85.5	4.145	4.044	4376.9	79.2	39.1
410	445	445	7.2	0.210	0.107	48.8	0.2	1.090	0.776	21.4	98.4	4.134	4.053	4683.5	79.0	41.9
420	445	445	7.2	0.234	0.107	51.2	2.5	1.092	0.776	19.6	81.2	3.800	3.726	4965.5	72.6	44.4
430	460	460	7.6	0.304	0.283	54.2	0.3	1.077	0.749	11.8	98.4	5.978	5.842	5409.0	114.3	48.3
440	460	460	7.6	0.330	0.054	57.5	-2.5	1.073	0.749	76.0	112.4	7.423	7.278	5959.7	141.9	53.3
450	460	460	7.6	0.321	0.051	60.7	1.7	1.078	0.749	63.9	90.8	5.834	5.720	6392.5	111.5	57.1
500	442	450	7.9	0.325	0.047	64.0	-3.4	1.037	0.714	89.5	117.2	7.612	7.443	6957.3	145.5	62.2
510	442	450	7.9	0.237	0.256	66.4	-2.7	1.043	0.714	12.3	119.5	5.667	5.597	7377.7	108.3	65.9
520	442	450	7.9	0.057	0.365	66.9	-1.8	1.055	0.714	2.8	159.3	1.822	1.787	7512.9	34.8	67.1
530	440	435	8.0	0.018	0.356	67.1	-1.8	1.028	0.827	1.6	286.8	1.033	1.013	7589.6	19.8	67.8
540	440	435	8.0	0.017	0.355	67.3	-2.7	1.027	0.827	2.1	404.4	1.345	1.318	7689.3	25.7	68.7
550	440	435	8.0	0.011	0.356	67.4	-1.1	1.029	0.827	1.0	298.8	0.633	0.621	7736.3	12.1	69.1
600	445	435	8.1	0.010	0.354	67.5	-0.8	1.419	1.245	1.0	298.5	0.611	0.599	7781.7	11.7	69.5
610	445	435	8.1	0.010	0.355	67.6	-1.0	1.419	1.245	1.1	352.8	0.722	0.708	7835.3	13.8	70.0
620	445	435	8.1	0.198	0.351	69.6	0.3	1.410	1.245	6.0	95.8	3.789	3.715	8116.4	72.4	72.5
630	450	440	8.8	0.156	0.350	71.1	1.5	1.013	0.791	4.1	82.6	2.578	2.528	8307.7	49.3	74.2
640	450	440	8.8	0.144	0.354	72.6	0.0	1.012	0.791	4.5	99.8	2.878	2.822	8521.2	55.0	76.2
650	450	440	8.8	0.171	0.351	74.3	-2.8	1.008	0.791	7.0	128.7	4.400	4.315	8847.7	84.1	79.1
700	447	438	9.1	0.111	0.349	75.4	2.9	0.999	0.776	1.8	50.1	1.111	1.090	8930.1	21.2	79.8
710	447	438	9.1	0.113	0.349	76.5	1.8	0.998	0.776	2.5	70.4	1.589	1.588	9048.0	30.4	80.9
720	447	438	9.1	0.075	0.349	77.3	2.0	1.000	0.776	1.1	48.2	0.722	0.708	9101.6	13.8	81.3
730	435	440	9.0	0.091	0.350	78.2	-1.3	0.989	0.764	3.6	124.1	2.300	2.255	9272.2	44.0	82.9
740	435	440	9.0	0.082	0.349	79.0	3.9	0.996	0.764	0.2	9.5	0.156	0.153	9283.8	3.0	83.0
750	435	440	9.0	0.108	0.348	80.1	-1.9	0.988	0.764	4.5	131.1	2.822	2.767	9493.2	53.9	84.8
800	440	440	9.1	0.168	0.348	81.8	1.6	1.077	0.860	4.3	81.0	2.722	2.669	9695.2	52.0	86.6
810	440	440	9.1	0.178	0.351	83.5	6.6	1.082	0.860	1.4	24.3	0.867	0.850	9759.5	16.6	87.2
820	440	440	9.1	0.204	0.000	85.6	6.9	1.081	0.860	0.0	32.1	1.311	1.286	9856.7	25.1	88.1
830	447	442	2.1	0.226	0.000	87.8	-6.8	0.785	0.814	0.0	126.9	5.723	5.611	10281.3	109.4	91.9
840	447	442	2.1	0.294	0.000	90.8	-8.8	0.778	0.814	0.0	125.1	7.367	7.224	10827.9	140.8	96.8
850	447	442	2.1	0.300	0.000	93.8	23.5	0.804	0.814	0.0	17.8	1.067	1.046	10907.0	20.4	97.5
900	440	440	1.8	0.262	0.000	96.4	26.0	0.710	0.712	0.0	8.1	0.422	0.414	10938.4	8.1	97.8
910	440	440	1.8	0.258	0.000	99.0	27.2	0.711	0.712	0.0	1.1	0.056	0.055	10942.5	1.1	97.8
920	440	440	1.8	0.152	0.000	100.5	16.0	0.711	0.712	0.0	1.1	0.033	0.033	10945.0	0.6	97.8
930	456	456	1.7	0.137	0.000	101.9	16.1	0.654	0.654	0.0	1.2	0.033	0.033	10947.5	0.6	97.8
940	456	456	1.7	0.139	0.000	103.3	16.3	0.654	0.654	0.0	1.2	0.033	0.033	10949.9	0.6	97.9
950	456	456	1.7	0.139	0.000	104.6	16.3	0.654	0.654	0.0	1.2	0.033	0.033	10952.4	0.6	97.9

Fig. 4. Graphical Output from Automatic Data Plotter--Pilot-plant Fluorinator

Computer programs based on PACER-65 have been used to calculate operating conditions from basic experimental data for both processing schemes. In this section, the program used for the O_2 - BrF_5 - F_2 processing cycle is outlined. The program for the O_2 - F_2 cycle involves calculations of the type described in the previous section for the pilot-plant fluorinator.

The major components of the experimental system used for studies of the O_2 - BrF_5 - F_2 cycle are the 2-in.-diameter fluid-bed reactor, soda lime traps for disposal of unreacted BrF_5 , lower bromine fluorides and uranium hexafluoride, a plutonium hexafluoride-collection system consisting of two sodium fluoride traps maintained at $100^\circ C$, activated alumina traps for disposal of fluorine, and a remote-head diaphragm pump. Figure 5 is a schematic diagram of the reaction system. These components are contained in an alpha glovebox and have been described in detail previously;⁹ supply manifolds outside the glovebox provide the process gases for the system.

Fig. 5. Fluorination Process Equipment--
Bench-scale Fluorinator

Approximately 20 v/o oxygen in nitrogen (as the inert fluidizing gas) is fed through the bottom of the reactor to oxidize the UO_2 - PuO_2 -F.P. pellets to U_3O_8 - PuO_2 powder. The fluidized-bed temperature is maintained at $450^\circ C$. During the BrF_5 selective fluorination step, 10 v/o BrF_5

in nitrogen is fed to the reactor, which is maintained at a temperature in the range from 200 to 400°C. The plutonium and traces of uranium remaining in the fluidized alumina bed are then converted to volatile hexafluorides by reaction with 90 v/o fluorine at 200 to 550°C. Since only small amounts of fluorine are consumed in this step, recycle of the reactant gases is employed to conserve the fluorine reagent. The fluorine off-gas from the reactor is passed through sodium fluoride traps for removal of hexafluoride products before being recirculated to the reactor by the diaphragm pump.

At regular intervals during an experiment, raw operating parameters for the reactor system are recorded; the parameters include system pressures, temperatures, and gas flow rates (either directly or as rotameter readings). These data are used as the input for the computer program which calculates the operating conditions which are reported. Gas flow rates are determined by the computer⁵ from calibration data for the rotameters, which give flow rate as a function of rotameter reading and system pressure.

For each set of data comprising reactor pressure, temperature, and gas flow rates, the following operating conditions are calculated for the three reaction steps:

Oxidation:

Total gas flow rate to pellet bed, liter/min
 O₂ concentration to pellet bed, v/o
 Total gas flow rate to fluidized bed, liter/min
 Superficial gas velocity--pellet bed, ft/sec
 Superficial gas velocity--fluidized bed, ft/sec

BrF₅ Fluorination:

Total gas to fluid bed, liter/min
 BrF₅ concentration to fluid bed, v/o
 Superficial gas velocity--fluidized bed, ft/sec

Recycle-fluorination with Fluorine:

Total gas to fluid bed, liter/min
 Superficial gas velocity--fluidized bed, ft/sec

The calculated results are printed as shown in Table 6. In addition to these printed results for each time interval of a given operation, a summary table is generated showing the operating conditions for the complete run. Table 7 is a typical example of this output. The summary table lists the type, size and weight of the fuel pellets, pellet-bed depth, pellet-bed support, fluid-bed material including size limits and static bed depth, as well as indicating the cumulative process time for the three process steps and the ranges of the corresponding operating variables.

TABLE 6. Computer Output Data Sheet--
Bench-scale Fluorinator

OXIDATION WITH O₂

TIME	REACTOR PRESSURE	GAS TO FLUID BED	VELOCITY FLUID BED	TEMP.	GAS TO PELLET BED	O ₂ CONC. PELLET BED	VELOCITY PELLET BED
0.0	970	16.0	0.78	450	14.8	21	0.72
0.5	970	16.1	0.78	452	14.8	21	0.72
1.0	980	16.1	0.78	450	14.9	21	0.72
1.5	1000	16.2	0.77	450	15.0	21	0.71
2.0	1000	16.2	0.77	450	15.0	21	0.71
2.5	990	16.2	0.77	452	14.9	21	0.72
3.0	990	16.2	0.77	452	14.9	21	0.72
3.5	1010	16.3	0.77	452	15.1	21	0.71

FLUORINATION WITH BRF5

TIME	REACTOR PRESSURE	GAS TO FLUID BED	VELOCITY FLUID BED	TEMP.	BRF5 CONC. FLUID BED
4.0	1210	25.1	0.64	202	10
4.6	1260	25.5	0.63	205	9
5.1	1290	25.8	0.63	205	9
5.6	1250	25.2	0.63	203	9
6.1	1270	25.4	0.62	202	9
6.2	1200	23.8	0.61	201	10
6.8	1200	24.6	0.64	202	10
7.0	1240	25.1	0.63	205	9
7.5	1140	24.1	0.66	205	10
8.0	1160	24.3	0.65	202	10
8.5	1110	23.6	0.66	201	10
9.0	1170	24.4	0.65	204	10

FLUORINATION WITH F₂-RECYCLE

TIME	REACTOR PRESSURE	GAS TO FLUID BED	VELOCITY FLUID BED	TEMP.
9.5	1190	15.3	0.40	204
10.5	1360	20.8	0.47	202
11.5	1420	21.4	0.47	202
12.5	1430	19.3	0.42	203
13.5	1455	20.1	0.47	252
14.5	1450	19.3	0.46	252
15.5	1290	17.4	0.51	301
16.0	1290	17.3	0.50	302
17.0	1400	22.0	0.59	302
18.0	1400	18.6	0.50	302
19.0	1420	19.3	0.54	330
20.0	1410	19.3	0.56	356
21.0	1455	20.7	0.66	437
22.0	1370	19.3	0.70	483
23.0	1360	19.3	0.75	532
24.0	1320	20.0	0.82	550
25.0	1350	20.0	0.80	550

TABLE 7. Summary Data Sheet--Bench-scale Fluorinator

AVERAGE OPERATING CONDITIONS FOR RUN PURSE-7

EQUIPMENT 2-IN. DIA. FLUID-BED REACTOR

UO₂-PUO₂ (+F.P.) PELLETS

SIZE 0.48-IN. DIA. X 0.41-IN. RIGHT CYLINDERS

WEIGHT 655.8 G

BED DEPTH 2-IN.

BED SUPPORT NICKEL BALLS

CSF ADDED 0.6 G

ALUMINA FLUID BED

MATERIAL ALCOA T-61 ALUMINA

SIZE LIMITS NOMINAL 48-100 MESH (-170 MESH FRACTION REMOVED)

WEIGHT 1100G

STATIC BED DEPTH 12-IN.

OXIDATION WITH O₂

CUMULATIVE PROCESS TIME (HR.)

0.0-4.0

REACTOR PRESSURE (MM HG)

970- 1010

TOTAL GAS FLOW TO FLUID BED (L/MIN)

16.0- 16.3

SUPERFICIAL VELOCITY (FT/SEC)

0.77- 0.78

OXYGEN CONCENTRATION TO PELLET BED (PERCENT)

21- 21

DILUENT

N₂

TEMPERATURE

450C

FLUORINATION WITH BRF5

CUMULATIVE PROCESS TIME (HR.)

4.0-9.5

REACTOR PRESSURE (MM HG)

1110- 1290

TOTAL GAS FLOW TO FLUID BED (L/MIN)

23.8- 25.8

SUPERFICIAL VELOCITY (FT/SEC)

0.61- 0.66

BRF5 CONCENTRATION TO FLUID BED (PERCENT)

9- 10

DILUENT

N₂

TEMPERATURE

200C

FLUORINATION WITH F₂-RECYCLE

CUMULATIVE PROCESS TIME (HR.)

9.5-25.5

REACTOR PRESSURE (MM HG)

1190- 1455

TOTAL GAS FLOW TO FLUID BED (L/MIN)

15.3- 22.0

SUPERFICIAL VELOCITY (FT/SEC)

0.40- 0.82

FLUORINE CONCENTRATION TO FLUID BED (PERCENT)

90

DILUENT

N₂

TEMPERATURE

200C, 9.5-12.5 HR
 250C, 12.5-15.5 HR
 300C, 15.5-18.5 HR
 300-550C, 18.5-23.5 HR
 550C, 23.5-25.5 HR

C. Application to Uranium-Plutonium Separation by Thermal Decomposition of Plutonium Hexafluoride

A 2-in.-diameter fluid-bed reactor system is being used to study the separation of plutonium from mixtures of uranium and plutonium hexafluorides. At temperatures of about 300°C at which uranium hexafluoride is stable, plutonium hexafluoride decomposes to solid plutonium tetrafluoride and fluorine.¹⁰ In this study, a bed of dense alumina is used to provide a surface for the decomposition reaction and for the deposition of the solid reaction product (PuF_4).

The thermal-decomposition flow system (see Fig. 6) consists of the hexafluoride and nitrogen feed systems, the 2-in.-diameter reactor, and primary filters, a secondary filter, the hexafluoride collection system, and alumina traps for fluorine disposal. This equipment and the glovebox enclosure have been previously described.⁶

Fig. 6. Process Equipment for Thermal Decomposition

The system is brought to operating temperature with nitrogen flowing. When the mixed hexafluoride gas stream is introduced, the nitrogen flow is reduced to permit maximum residence time of the gas in the fluid bed. Solid plutonium tetrafluoride formed by decomposition deposits on the particles of the bed. The fluorine from the reaction and the uranium hexafluoride pass to the collection system, where the uranium hexafluoride is condensed. Careful control of flow rates is maintained to ensure good bed fluidization at minimum flow rates.

The data-reduction program utilizes data for flow rates, temperatures, and pressures taken during the run together with other input information such as orifice calibrations, changes in bed weight due to sampling, and bed properties. Operating conditions are calculated for each 30-min interval as follows:

Bed weight, g
 Bed height, in.
 Bed temperature (low, high, and average), °C
 Gas residence time, sec
 Inlet and off-gas pressures, psia
 Flow rates, g/min or scfm
 Hexafluoride concentration, v/o
 Superficial gas velocity, ft/sec
 Filter pressure drop, psi
 Bed density, g/cc

Typical results are shown in Table 8. The results are also summarized in a table of average conditions for the total run period, as in Table 9. Separate summaries of portions of the run may be obtained if desired. Graphs are prepared showing hexafluoride concentration and gas residence time as a function of run time (see Fig. 7). The tables and graphs can be readily reproduced for direct use in reports as in the above examples.

Fig. 7. Graphical Output from Automatic Data Plotter--
 Thermal Decomposer

TABLE 8. Computer Output Data Sheet--Thermal Decomposer

RUN TIME (HOURS)	BED WEIGHT (GM)		BED HEIGHT (IN)	BED TEMPERATURE (DEGREES C)			GAS RES. TIME (SEC)	PRESSURE (PSIA)		HEX RATE (G/MIN)	FLOW RATES (SCFM)		VOLUME PERCENT HEX	SUP. VELOCITY (FT/SEC)	FILTER DP (PSI)	BED DENSITY (G/CC)
	CALC	MEAS		LOW	HIGH	AVE.		INLET	OFF-GAS		N2	TOTAL				
0.00- 0.50	2319	1460	18.3	294.0	299.0	296.5	7.7	15.3	14.3	14.8	0.1075	0.1409	23.7	0.202	0.480	1.45
0.50- 1.00	2319	1460	18.3	294.0	299.0	296.5	7.7	15.3	14.3	14.8	0.1075	0.1409	23.7	0.202	0.528	1.45
1.00- 1.50	2319	1460	18.3	292.0	298.0	295.0	8.0	15.3	14.3	14.8	0.1075	0.1409	23.7	0.201	0.528	1.42
1.50- 2.00	2319	1460	18.3	288.0	295.0	291.5	8.3	15.3	14.3	14.8	0.1075	0.1409	23.7	0.200	0.528	1.38
2.00- 2.50	2319	1460	18.3	290.0	299.0	294.5	8.5	15.3	14.3	14.8	0.1075	0.1409	23.7	0.201	0.528	1.35
2.50- 3.00	2319	1460	18.3	291.0	299.0	295.0	12.8	15.3	14.3	17.6	0.0611	0.1007	39.4	0.144	0.528	1.29
3.00- 3.50	2319	1460	18.3	294.0	299.0	296.5	12.4	15.3	14.4	22.3	0.0611	0.1113	45.1	0.160	0.528	1.23
3.50- 4.00	2319	1460	18.3	293.0	298.0	295.5	12.4	15.1	14.4	22.2	0.0609	0.1109	45.0	0.160	0.528	1.23
4.00- 4.50	2319	1460	18.3	290.0	298.0	294.0	12.4	15.1	14.4	22.2	0.0609	0.1109	45.0	0.160	0.528	1.23
4.50- 5.00	2183	1460	17.3	290.0	298.0	294.0	11.7	15.1	14.4	22.2	0.0609	0.1109	45.0	0.160	0.504	1.23
5.00- 5.50	2183	1460	17.3	289.0	300.0	294.5	11.6	15.0	14.4	22.1	0.0608	0.1105	45.0	0.161	0.528	1.23
5.50- 6.00	2183	1460	17.3	287.0	301.0	294.0	11.3	15.0	14.4	23.2	0.0608	0.1129	46.2	0.164	0.552	1.23
6.00- 6.50	2183	1460	17.3	284.0	305.0	294.5	11.5	15.3	14.5	23.4	0.0611	0.1137	46.3	0.162	0.528	1.23
6.50- 7.00	2183	1460	17.3	275.0	301.0	288.0	11.5	15.1	14.8	23.3	0.0609	0.1133	46.2	0.162	0.528	1.23
7.00- 7.50	2183	1460	17.3	277.0	299.0	288.0	10.5	15.0	14.7	23.2	0.0708	0.1229	42.4	0.177	0.528	1.23
7.50- 8.00	2183	1460	17.3	276.0	292.0	284.0	10.4	14.5	14.4	22.8	0.0703	0.1217	42.2	0.179	0.480	1.23
8.00- 8.25	2183	1460	17.3	294.0	296.0	295.0	13.9	15.0	14.4	9.5	0.0708	0.0921	23.1	0.134	0.384	1.23

TABLE 9. Summary Data Sheet--Thermal Decomposer

CONDITIONS OF THERMAL DECOMPOSITION RUN DUP-5

EQUIPMENT	2 IN. DIAMETER REACTOR	SUPERFICIAL VELOCITY (FT/SEC)	0.17
FEED	UF6-PUF6	TOTAL FLOW RATE (SCFM)	0.120
BED MATERIAL	ALCOA T-61 -100 MESH ALUMINA	N2 RATE (SCFM)	0.076
		HEX. FEED RATE (GM/MIN)	19.6
BED WEIGHT (GM)	2257	HEX. CONCENTRATION (V/O)	37
BED HEIGHT (STATIC) (IN)	17.8	TOTAL HEX. PROCESSED (GM)	9707
BED TEMPERATURE (C)	293	RUN DURATION (HRS)	8.25
REACTOR INLET PRESSURE (PSIA)	15.2		

IV. CONCLUSIONS

The generalized computer program PACER-65 is a useful method for the calculation of flowsheet data; the effects of flowsheet modifications and variations in processing conditions are readily evaluated. Adaptation of PACER-65 for process-data reduction has provided a systematic method for the calculation of operating conditions from the raw experimental data recorded during a process run. Use of the PACER-65 method in additional flowsheet studies and data-reduction applications is recommended.

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