Fixed Bed Reactor Design Program Development Based on Java

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Abstract—**A fixed bed reactor design program is developed by the use of Java JDK1.7 algorithm language with Eclipse program as the platform. The program selects five common fix bed reactor process flows to calculate the main structure parameters of the reactor. With the good interface, the program can output the corresponding results after inputting the kinetics and thermodynamics parameters of the reaction process. The result has little error compared with that of the real industrial device. The program can be applied in scientific research, engineering design and teaching.**

Index Terms—**java language, program, fixed bed reactor , design**

I. Introduction

Fixed bed reactor is a kind of gas-solid catalytic reactor which is mature is in application and research in the petrochemical production process. Its design plays a vital role in the whole production process. The undesirable reactor will lead to low reaction conversion rate and poor selectivity and even cause accidents due to the runaway of the reactor. The type and internal structure of the fixed bed reactor vary according to the type of catalyst and chemical reaction. so it's a typical non-standard equipment that needs to make corresponding designs according to different production processes. And, the design process is very complex, including the contents of many disciplines like chemical engineering, mechanical engineering, chemical engineering principle and thermodynamics, so many factors need to be taken into account. [1-4]

This program selects several common fixed bed reactor production processes and designs the main structure of the reactor. The object-oriented Java SE algorithm language in Version Java JDK1.7 and the Eclipse program are used in the program development.

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A. Technical Advantages of Java SE and Eclipse

At present, Java2 has three versions, in which Java SE is short for Java platform standard edition. Java language is an object-oriented design language. The object-oriented programming is based on the concept and abstraction of the structured programming, mainly including object, class and inheritance. Object refers to the entity formed by the data describing its properties and all operations imposed on these data . Objects can link to each other only through delivering passage. Java language design focuses on object and its interface. It provides the simple class mechanism and the dynamic interface model. Its state variables and the corresponding method are packaged in objects, thus realizing modularity and information hiding; class provides the prototype of a class of objects. And, the subclass can realize the method of the parent class to realize the method reuse through the inheritance mechanism. For example, in the display of realizing the interface window, the classes of all windows are inherited from JFrame Class to realize the interface function in Java SE; in label and button realizing the monitoring function, ActionListener interface and mouse or keyboard monitoring are realized; in addition, in algorithm implementation, the data encapsulation is realized to avoid the possibility that the external class changes the internal data of algorithm. The object-oriented design makes the use of abstract concepts in the program more reasonable. And, the object-oriented design method establishes a higher level of abstraction than the traditional ones. In object orientation, process and data are combined to form the entity of object. The description of a group of similar objects is class. The instance of class is the real objects it describes. The further abstraction can be realized by using the class hierarchy. In order to reuse the previously defined methods, class hierarchy educes the inheritance mechanism in object orientation. [5-7]

Eclipse is an integrated environment supporting a variety of development languages. With the advanced plug-in management system, it can extend its functions according to its own requirements through plug-in. Now the plug-ins supporting almost all popular languages

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including C, C++, Python and PHP are available. Eclipse integrates Java development plug-in by default and the programming of this system is based on the Eclipse platform.

Eclipse has the cross-platform characteristic of Java and can run on almost all operating systems.

Fig.1 is the screenshots that Eclipse is compiling Java project under the win 7 system.

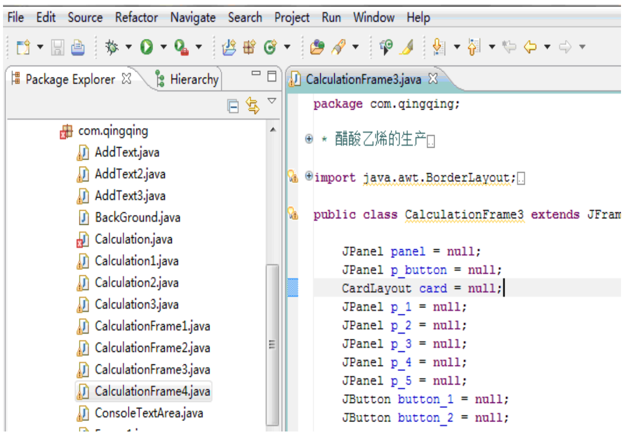

Figure1. The Running Eclipse Compiler.

B. Programm Introduction and Function Analysis of the System

The program is written with Java1.7.0 language. Java program shows the strong cross-platform characteristic in running, so this program does not require strict hardware and system support, but can be debugged after installing Java virtual machine in the operating system.

Considering the users and the development cycle of this program, fast prototype method is used to develop the design system. Through the rapid analysis , the users and the designers' requirements are determinined. Then after structuring the prototype, the initial prototype system is developed, and the prototype can be used and evaluated by the users and the system developers; finally system developers modify and perfect the prototype system. [8]

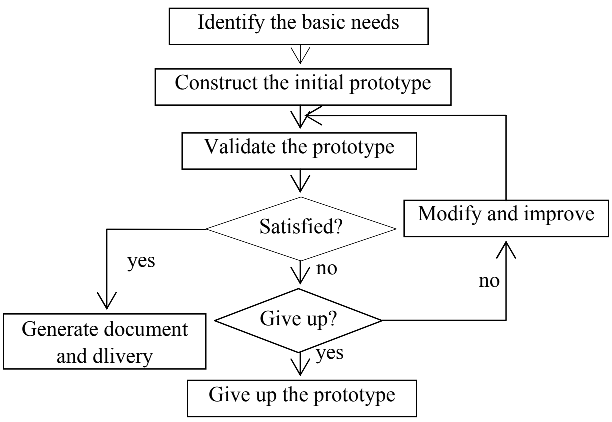

Figure2. Fast Prototype Method.

The program can be divided into three modules according to the function: data input module, preliminary design module and internal component module. Data input module corresponds to the receipt of the original data, including the receipt of the data of the preliminary design and the internal component. It's based on the initial design conditions, but requires providing the necessary suggestions on the designer's input and modification; preliminary design module corresponds to structure calculation and preliminary design scheme determination. It uses the cyclic iterative method to solve the differential equation to obtain the preliminary design parameters; internal component module mainly selects and designs internals of the reactor and stores the data of the main standards. The storage of the standard data can reduce the designer's workload of querying the standard specification.

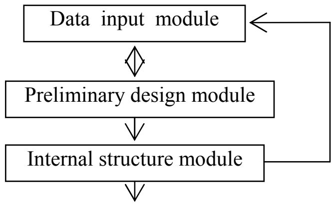

Figure3. System Structure.

With the Eclipse as platform, process flow selection interface is loaded by developing program in Java language. And then the initial datas are written the input interface and the design and checking program according to different technological processes in order to get basic data.

There is option of traditional process parameters in the program for convenient for inputting datas. And the parameters can be determined by choosing the traditional technological process. Finally, according to the basic data, type selection and design of parts in reactors are completed. In the process of programming, each reaction model is designed as a separate module; each module can be analyzed separately according to different techno-logical characteristics. So the applicability of the program can be improved greatly.

C. Program Interface Composition

The underlying data interface function is developed to realize the input of external data. Then, the external data are transmitted to the calculation module through the space array.

This program is written with Java J2SE interface programming technique. All Windows are inherited from the Jframe class with strong reusability and clear composition.

In the input window, the reusability of the window is enhanced through the method of parameter passing. For instance, when designing the tube heat exchange-type fixed bed reactor, the constructor code of the form is as follows:

public CalculationFrameExchange(String str) throws HeadlessException{…

Make judgment in the program. When the parameter is the fixed bed reactor design of oxidation of o-xylene to phthalic anhydride, it's passed to the data of oxidation of o-xylene to phthalic anhydride with the following code:

```
if (str == "The fixed bed reactor design of oxidation of o-xylene to phthalic anhydride") {
new Parameters("raw material ratio w% (air： o-xylene)： ", p_2, 0, 280);
new AddText2(p_2, T, "480", 0, 70);
new AddText2(p_2, P, "1000", 0, 190);
new AddText2(p_2, null, "8.5： 1.5", 0, 310);
new AddText2(p_2, Sv, "3000", 350, 70);
new AddText2(p_2, x, "80%", 350, 190);
new AddText2(p_2, u0, "300", 350, 310);            }
```

By this way, it enhances the reusability of the form and simplifies the structure.

The design results are divided into two parts. First of all, in the design process, it shows partial results in the design to the designer in the way of capturing the output stream of the console, so that the designer can adjust the set parameters timely and thus optimize the design. The code that realizes this method uses a class. With the multithread advantage of Java, it controls the output thread of the console and presents the output content in JtextField to display it in the form, thus making the results more clear.

The second kind of result presentation is realized after the completion of design. It's output in the PDF table to present the input design parameters and the final design results. All design input and output parameters are listed in the table. The program realizing this method uses an itext expansion pack of open source to draw the output result table in the PDF file.

Part of the source code generating PDF documents are as follows:

```
//Create a A4 paper size document
Document document = new Document(PageSize.A4);
try {
//Create a listening for the document, and write PDF stream to the document.
PdfWriter.getInstance(document,newFileOutputStream("d:\\PDFDocument.pdf"));
//Open document
document.open();
//Add the text
Paragraph word = new Paragraph(str, fontCN);
word.setAlignment(1);
document.add(word);
//Create a table of four columns
float[] widths = { 20f, 20f, 30f, 30f};
table = new PdfPTable(widths);
//Define a table cell
cell=newPdfPCell(new Paragraph("Design Parameter", fontCN));
//Define the span of a table cell
cell.setColspan(3);
//Add the cell into the form
cell.setHorizontalAlignment(Element.ALIGN_CENTER)
cell.setVerticalAlignment(Element.ALIGN_MIDDLE);
table.addCell(cell);
```

D. Computation Module of the Program

In the computation module, the iterative algorithm is used to solve the equation; then the rationality analysis is made within the computation to finally form the preliminary design scheme. After that, the preliminary design scheme of the obtained fixed bed reactor is used to make the type selection and checking of components and then obtain the final design scheme. The advantage of this calculation method is that the modularized design method enhances the scalability of the program and makes it have strong compatibility and portability, which is convenient for program maintenance and function expansion function. At the same time, the program runs faster.

II. Mathematical Model of the Fixed Bed Reactor Design [9-17]

The mathematical model used in this program is the pseudo-homogeneous one-dimensional model which ignores the influence of the bed axial dispersion and further simplifies the bed to be the pseudo-homogeneous plug flow reactor.

A. The External Radial Heat Exchange Item of the Bed

The heat transfer performance of the bed has great influence on the temperature distribution in the bed as well as the reaction rate and material component distribution. Since the reaction is carried out within the catalyst particles, the heat transfer of the fixed bed essentially includes heat transfer within particles, between the particle and the fluid and between the bed and the wall. The catalyst in the fixed bed catalytic reactor is often a poor conductor of heat, and the solid particle is large with poor heat conduction performance. As a result, the heat transfer performance of the bed is poor. In addition, the complex temperature distribution is formed in the bed. In the reactor, not only the axial temperature distribution in the reactor is uneven, but also the radial temperature has the temperature gradient. This program just involves the pseudo-homogeneous one-dimensional reaction model, and all calculations ignore the axial temperature transfer and assume the bed to be the piston flow.

The external radial heat transfer equation is shown as (1).

where

$$q = \alpha_w (T - T_w) \quad (1)$$

q — Heat transfer flux, W/m^2

α_W—Convective heat-transfer coefficient of the reactor wall, $W/(m^2 \cdot K)$

T—Reaction temperature, K

T_W—Temperature of the reactor wall, K

The heat transfer coefficient α_W of the catalyst bed and the reactor wall can be calculated with (2).

$$\frac{\alpha_w \times d_i}{\lambda_g} = 3.5\left(\frac{d_p \cdot u \cdot \rho_g}{\mu_g}\right)^{0.7} \cdot \exp\left(-4.6\frac{d_p}{d_i}\right) \quad (2)$$

where

d_i —Interior diameter of the reactor, m

d_p —Diameter of catalyst particle ,m

λ_g —Coefficient of heat conductivity of the gas through the bed, $W/(m^2 \cdot K)$

μ_m —Viscosity of the gas ,*kg/m·s*

u —Line velocity of the gas, *m/s*

ρ_g —Density of the gas passing through the bed, kg/m^3

B. Intrinsic Kinetics Equation

The gas-solid phase catalytic reaction process often consists of adsorption, reaction and desorption. Due to the different equation types of the adsorption rate, the intrinsic kinetics equation also has different forms.

Take the reaction process of synthesizing ethylene vinylacetate(VAC) by ethylene process as an example. Its intrinsic kinetics equation is:

Where

$$r_A = \eta_e k_0 \exp\left(\frac{-E}{RT}\right) f\left(y_{VAC}\right) \tag{3}$$

r_A—Formation rate of Component A, *mol/(kg.h)*

η_e —Effectiveness factor of catalyst

k_0—Pre-exponential factor of the reaction

E—Reaction Activation energy, *J/mol*

R—Mole gas constant ,*J/(mol.K)*

$f(y_{VAC})$ —Function of VAC mole fraction

$$f\left(y_{VAC}\right) = y^0_{O_2} + 1.5y^0_{CO_2} - 1.5y_{CO_2} - 0.5\left(1 - y^0_{O_2} - 1.5y^0_{CO_2}\right)y_{VAC} \tag{4}$$

C. Mass Transfer in the Fixed Bed Reactor

The mass transfer process in the fixed bed reactor includes external diffusion, internal diffusion and mixing diffusion in the bed. As the gas-solid phase catalytic reaction occurs mainly on the surface of catalyst, the reaction components must reach the surface of catalyst to realize the chemical reaction. Therefore, the reaction mainly occurs in the inner surface and the internal diffusion process directly affects the macro rate of the reaction.

The concentration distribution equation of the bed is:

$$\left(\frac{dw_A}{dl}\right) = \left(\frac{A_r}{G}\right) r_A \rho_B \tag{5}$$

Where

w_A—Mass fraction of component A

l—Height of the bed,m

A_r—Cross section of the reaction bed, m^2

G—Mass flow of raw mix, *kg/h*

ρ_B— Packing density of the reaction bed, kg/m^3

D. Temperature Distribution Equation

$$G\bar{C}_p\left(\frac{dT}{dl}\right) = A_r r_A \rho_B\left(-\Delta H_r\right) - \frac{d}{l}q \tag{6}$$

Where

$\bar{C}_p$ —Average mass heat capacity at constant pressure of the reaction material,*J/(kg.K)*

$-\Delta H_r$ —Reaction heat, *J/mol*

E. Design Framework

The calculating steps of the design module of the fixed bed reactor is shown in the below block diagram.

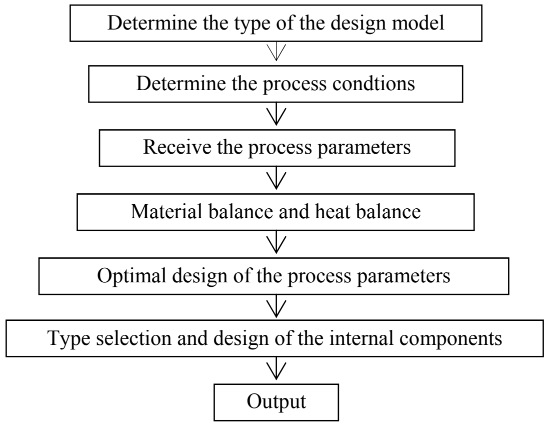

Figure4. Block Diagram.

III. REACTOR STRUCTURE DESIGN [11-14]

A. Size of Tube Bundle and Arrange of Reaction Tube

The diameter of the tubular fixed bed reactor is mainly restricted by different responses themselves. The tube diameter of the strong exothermic reaction or strong endothermic reaction is generally as small as 20 mm to 30 mm.

According to the inner diameter of the tube, the volume of the single-tube catalyst is:

$$V_1 = \frac{1}{4}\pi d^2 l \tag{7}$$

where

V_1—The volume of the single-tube catalyst, m^3

d —Inner diameter of the tube,m

Then, the quantity of the tubes n is:

$$n = \frac{V_R}{V_1} \tag{8}$$

where

V_R—The volume of the catalyst bed, m^3

$$V_R = \frac{V_0^\theta}{S_V} = \frac{22.4 \times F_{t0}}{S_V} \tag{9}$$

where

F_{t0}—The total gas flow rate entering into the reactor, *kmol/h*

S_V— Space velocity, h^{-1}

V_0^θ—The standard volume flow rate entering into the reactor, m^3/h

The layout of the reactor shell and tube is quite different from that of the ordinary heat exchanger. It has the following characteristics: the water circulation in the central tube bundle is blocked, resulting in deterioration of heat transfer and uneven temperature distribution, so there is no tube layout in this area.The reaction tube calandria divides the whole tube sheet into 12 intervals by 30°. The whole tube sheet is composed of an array at the interval of 30°.

Therefore, the users need to determine the diameter of the central no-tube-layout area according to different capacities and the effective cross-sectional areas of the reactor bed. It's generally between 200 mm to 1000 mm.

Then different arrangement forms are chosen to determine the tube pitch and calculate the area occupied by the single pipe; after that, the diameter of the reactor is determined according to the number of tubes. If the diameter is too large, it's considered to divide the reactor into several parts in parallel.

The tubes are arranged mainly in the equilateral triangle, so it's not specified in this program. All are arranged in the equilateral triangle as shown in Fig.5.

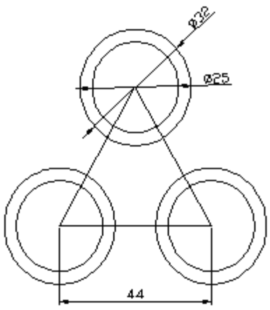

Figure5. The Diagram of the Reactor Tube Arrangement.

Tube pitch usually takes 1 to 2 times of the outside diameter of the tube.

With the triangle arrangement, the area occupied by the single tube is:

$$s=\frac{\sqrt{3}}{2}t^2 \tag{10}$$

Then, the diameter of each reactor is:

$$D_i=\sqrt{\frac{\frac{n}{m}\times s+\frac{1}{4}\pi d_i^2}{\frac{1}{4}\pi}} \tag{11}$$

Where

D_i—The diameter of each reactor, *m*

n—Tube quantity

m—Number of reactors

s—The area occupied by the single tube, m^2

d_i—The diameter of the central non-tube-arrangement area, *m*

B. Reactor Bed Pressure Drop

The pressure drop of the fixed bed passed by the fluid is mainly caused by the frictional resistance between the fluid and the particle surface and the shrinkage, expansion and redistribution of the fluid in the channel. When the flow is stranded, the pressure drop is mainly caused by the frictional resistance; when the flow is turbulent, it's mainly caused by local resistance. Many formulas can be used to calculate the pressure drop. The commonly used one is Ergum formula which is derived from the pressure drop formula of the fluid flowing in the hollow tube.

$$\frac{\Delta p_b}{H}=f_m\frac{\rho u_0^2}{d_p}\left(\frac{1-\varepsilon_b}{\varepsilon_b}\right) \tag{12}$$

$$f_m=a+b\left(\frac{1-\varepsilon_b}{R_{sm}}\right) \tag{13}$$

$$R_{sm}=\frac{d_p\rho u_0}{\mu}. \tag{14}$$

where

ΔP_b—Pressure, *Pa*

f_m—The modified coefficient of friction

ρ—The fluid density, kg/m^3

u_0—Superficial linear velocity, *m/s*

d_p—Diameter of the catalyst particle,*m*

ε_b—Bed voidage

H—Bed height, *m*

μ—Absolute viscosity of the fluid, *Pa.s*

a、b—Coefficient, adopt the values proposed by Ergun, a=1.75, b=150.

IV. Analysis of the Reactor Design Results

Optimizing analysis is conducted on the main structure size of the reactor in different processes. Next, the oxidation of o-xylene to phthalic anhydride is taken as an example to analyze and discuss the design result.

A. The Change of O-xylene Conversion Rate with Different Lengths of the Tube

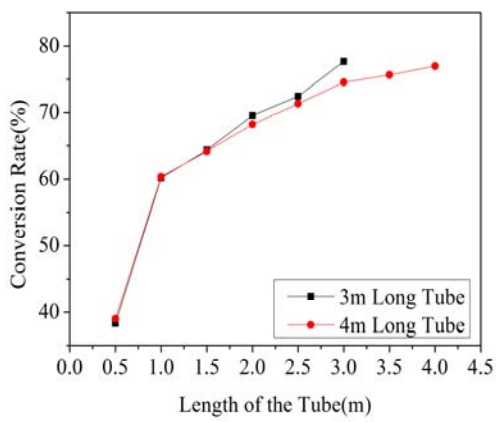

Figure6. The Change of O-xylene Conversion Rate with the Tube Length.

It can be seen from Fig.6 that the conversion rate of the reactor with the 3m long tube is significantly higher than that with the 4m long tube. It's mainly because that the flow resistance of the 4m long tube is large.

B. The Change of the Bed Temperature When Adopting Diffrent Raw Material Proportions

A 3m long tube is chosen with the inlet temperature at 370 ℃ to investigate the bed temperature change when air/o-xylene are 8.5/1, 9.5/1 and 10/1, respectively, as shown in Fig.7.

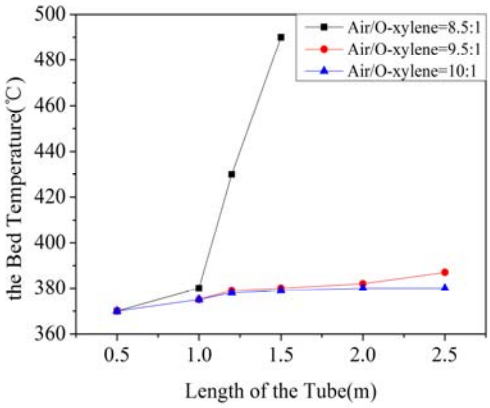

Figure7. The Bed Temperature Change with the Raw Material Proportion.

According to Fig.7, when air/o-xylene is 8.5/1, the temperature at 1.5 m of the bed is about 490 ℃, 120 ℃ higher than the feed temperature, indicating the temperature runaway phenomenon in the bed. And when air/o-xylene is 9.5/1 or 10/1, the reactor operates smoothly.

After the preliminary optimization design, the final design conditions of five kinds of processes are determined.

C. *Design Result Analysis of Five Kinds of Processes*

In computation, water/hydrocarbon for the ethyl-benzene dehydrogenation reaction is 2.2/1. Oxidation of o-xylene to phthalic anhydride adopts the low air ratio method with air/o-xylene of 9.5:1. The feed gas of the methanol synthesis reactor is composed of $H_2$76%, CO7%, $CO_2$2%, CH_4+$N_2$13.4%, CH_3OH0.4% and H_2O0.2%. Ethylene oxide takes silver as catalyst and the compositions of the mixture are $H_2$74.22%, N_2 24.74%, $CH_4$0.75% and A_r 0.29%. The main process conditions are shown in Table Ⅰ.

The design structure size and the actual size of the reactor in five kinds of processes are shown in Table Ⅱ. It can be seen from the table that there is no great difference between the design value and the actual one.

V. CONCLUSION

A fixed bed reactor design program is developed with the Java language to design the main structure sizes of several typical chemical production processes. With the good man-machine interface, the program gives hints and instructions to the user in the using process, which can guide the operation process. The implementation of the program summarizes various design processes of the fixed bed reactor to realize the integration of the design process, which facilitates the user's overall design.

For the programming modularization, both type selection and design are divided into different subprograms according to different process reactions and different part functions. Each subprogram finishes the specified work for flexible application, extension and maintenance.

This program adopts the pseudo-homogeneous one-dimensional model to design the computed tubular reactor. Tubes of different lengths and diameters and different heat transfer forms can be selected for calculation.

Under the same process conditions, the design value of

TABLE II.
MAIN OPERATING PARAMETERS OF FIVE KINDS OF PROCESSES

	Ethylbenzene Dehydrogenation	Methanol Synthesis	Phthalic Anhydride	Vinyl Acetate	Ethylene Oxide
Output,kt/a	20	500	40	100	240
Inlet temperature,℃	630	225	370	175	210
Outlet temperature,℃	-	254	385	-	250
Inlet pressure,MPa	-	8.0	0.1013	0.784	1.0
Outlet pressure,MPa	630	225	370	175	210

TABLE I.
DESIGN RESULT

	Ethylbenzene Dehydrogenation		Methanol Synthesis		Phthalic Anhydride		Vinyl Acetate		Ethylene Oxide	
	Design Value	Actual Value	Design Value	Actual Value	Design Value	Actual Value	Design Value	Actual Value	Design Value	Actual Value
Tube inner Diameter,mm	100	100	34	34	28	25	27	27	27	24.5
Tube Height,m	3	3	6	6	3	3	10	10	8	8
Tube Number	7600	7421	6856	6713	21013	20505	7923	7860	9217	8821

the program shows little difference with the actual value of the factory reactor.

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