APPLICABILITY OF CHEMICAL GETTER BEDS TO SCAVENGE TRITIUM FROM INERT GASES

Jon L. Matenschein

March 10, 1976

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*Work performed while LLL summer employee. Author now at Chemical Engineering Department, University of California, Berkeley.

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APPLICABILITY OF CHEMICAL GETTER BEDS TO SCAVENGE TRITIUM FROM INERT GASES

Abstract

Chemical getters can be used to scavenge tritium from inert gases. Cerium - which forms a hydride with a low dissociation pressure, has high reactivity, and is relatively inexpensive - is a good candidate getter material for such a scavenger system. Mathematical models for using cerium in both fixed- and fluidized-bed reactors predict satisfactory

performance. Moreover, the capital cost of a gettering system, estimated to be between \$115,000 and \$166,000 (m^3/s) flow, is competitive with that of the conventional catalytic-oxidation molecular-sieve system (\$330,000/ m^3/s) now used. The gettering concept, therefore, warrants further investigation. This report assesses the feasibility of such a system.

Introduction

The removal of tritium from inert gases has two important controlled thermonuclear reactor (CTR) applications:

- Scavenging tritium from the atmosphere of a room contaminated by a spill (at room temperature and pressure)
- Routine removal of tritium from blanket coolant gases (at high temperature and pressure).

The tritium-removal process traditionally used is to oxidize the tritium to water catalytically, and

then adsorb the water using a molecular sieve.^{1,2} This approach, however, involves a high capital cost and converts tritium from T_2 gas to the more hazardous T_2O form.

A logical alternative is to use a chemical getter to absorb the tritium directly. Direct absorption would eliminate the production of undesirable T_2O . In addition, a getter system might use fewer or cheaper materials and, therefore, be less expensive.

This report assesses the feasibility of such a chemical getter system. The major steps in this study were to:

- Select a getter
- Mathematically model the getter process
- Study different reactor types for use with the getter
- Conceptually design a prototype reactor and system
- Estimate the capital cost of such a system for comparison with the traditional catalytic-oxidation approach.

SYSTEM PERFORMANCE PARAMETERS

The major emphasis of the study was on evaluating the feasibility of a getter system to clean up spills in a reactor working space. To compare the getter system with the catalytic-oxidation system, the following guidelines were established:

- A volume of $21,600 \text{ m}^3$ is contaminated with 21.6 gm of T_2 , making the initial tritium level 10 Ci/m^3 (3.8 ppm).*
- After 24 hr of purification, the tritium level must be down to $500 \text{ } \mu\text{Ci/m}^3$. (Assuming 40 volume changes may be

necessary to achieve this reduction because of surfaces adsorbing and desorbing tritium³ gives a system-flow requirement of $10 \text{ m}^3/\text{s}$.)

- The contaminated volume contains only argon and tritium. The effects of impurities are considered only qualitatively.

The system is conceived as one that should run for a short time (e.g., 24 hr) to clean up spills. Using a getter system to recover tritium from blanket coolant gas would require a continually operating process: one case would require recovery of about 7 g/day of tritium from a helium stream with a tritium concentration of 0.223 ppm^2 .

GETTER SELECTION

Desirable getter characteristics include:

- Low dissociation pressure of tritium
- High reactivity (i.e., fast reaction between tritium and the getter)
- Large tritium capacity
- Low cost and good availability
- Resistance to poisoning.

In screening potential getters, the dissociation hydrogen pressure over the hydride was the major factor

*This volume is about one-sixteenth that needed to house a fusion-fission hybrid reactor.² A system of any required capacity can be obtained by using several getter systems in parallel, as appropriate.

considered. Dissociation pressures for potential getters are shown in Fig. 1 as a function of temperature, with an equation for each line.* For most getters, dissociation-pressure data exist only for high temperatures. Extrapolation to lower temperatures may introduce errors, but provides the best estimates at present. These equations were derived from data in the literature.⁴⁻⁷⁴ The getters with the lowest dissociation pressures for temperatures between 25 and 250°C were yttrium,^{4,6,22,27,65-70} erbium,^{4,6,22,27,59} scandium,^{4,6,22,27,63-65,72} and cerium.⁴⁻²⁷ Uranium has been studied extensively,^{4,28-37} but has a higher dissociation pressure.

Tritium capacity (kg T₂/kg getter) at the upper composition limit of the pressure plateaus is reasonably similar for all four getter materials, except scandium, which has about twice as much capacity as the others due to its low molecular weight.

Of the four getters, cerium is the cheapest and most abundant, with production in ton quantities being

common.²⁷ The other getters - yttrium, scandium, and erbium - are either significantly more expensive, less abundant, or simply not as well characterized. For these reasons, cerium metal was chosen as the getter material for this study. Some physical properties of cerium and cerium hydride are given in Table 1.

Cerium is not without drawbacks. The data for dissociation pressures were taken between 500 and 800°C - liberal extrapolation is necessary to predict pressures close to room temperature. Cerium is highly reactive and pyrophoric in air. Cerium also reacts with nitrogen, carbon monoxide, carbon dioxide, and water. Because of this high reactivity, poisoning could prove troublesome. These are also likely characteristics of the other getter materials, but are not considered to be crucial for the purposes of this study.

A possible alternative to using pure cerium would be to use mischmetal - a mixture of rare earths, predominantly cerium. It costs less and the dissociation pressures of hydrided mischmetal²⁵ appear to be comparable to those of a hydrided cerium. This is to be expected, since the rare earths found in mischmetal have hydride dissociation pressures similar to cerium.^{6,12,15}

*Other getters considered, but not included in Fig. 1 were Th₂Al, Zr, Hf, Ba, Ti, and TiZr.

Fig. 1. Dissociation pressures of metal hydrides versus temperature.

Table 1. Properties of cerium (Ce) and cerium hydride (CeH₂).

	Ce	CeH ₂
Molecular weight	140	142
Density (g/cc)	6.7 ^a	5.4 ^{b,c}
Melting temperature (°C)	799 ^a	1080 (for CeH ₃) ^d
Specific heat at 25°C (J/kg K)	192 ^a	
Hydrogen capacity of Ce (as CeH ₂)		0.014 kg H ₂ /kg Ce 0.041 kg T ₂ /kg Ce
Equilibrium pressure of CeH ₂ (T in K, P in torr)		$\log_{10} P = 10.72 - 10840/T^{e,f}$
Heat of reaction: H ₂ + Ce → CeH ₂	$\Delta H = -202 \text{ kJ/mol}$ -206 kJ/mol	650°C ^e 25°C ^f

^aSee Ref. 75.^bSee Ref. 23.^cSee Ref. 26.^dSee Ref. 8.^eSee Ref. 11.^fSee Ref. 12.

The Gettering Process

DESCRIPTION

The gettering of tritium occurs in several steps:

- Tritium diffuses from the gas to the getter surface

- Tritium molecule dissociates to form atoms on the getter surface
- Tritium atoms diffuse through a layer of tritided getter to reach untritided material

- Tritium atoms react with untritided getter.

A model of the gettering process depends, of course, on which step controls the rate. Unfortunately, the controlling step is not yet known.

The reaction rate of tritium (or hydrogen) with cerium is not known; even that of hydrogen with uranium is subject to considerable disagreement.⁴ It is also difficult to predict the rate of diffusion of tritium atoms in the tritide layer and the rate of tritium dissociation on the surface.

As cerium is hydrided, it tends to flake and spall^{9,10} because of the volume change induced by hydriding (see Table 1). This has the effect of continually exposing fresh surface. Therefore, diffusion through the tritide layer is not likely to be the controlling step.

The rate of diffusion in the gas phase can be predicted from mass-transfer theories as well as from empirical correlations.

In deciding which step to treat as rate-determining, the dissociation of the tritium molecule to atoms and the diffusion of the tritium atoms through the solid tritide (with the spalling effect) were both assumed to be rapid. These assumptions were

necessary because of the lack of rate data for either step. The reaction of hydrogen with cerium is similar to the reaction of hydrogen with uranium in that the two reactions are thought to have similar mechanisms (both hydrides are very stable, the cerium hydride being more stable than the uranium hydride, and both exhibit plateau regions). Therefore, because the uranium-hydrogen reaction is rapid, it is reasonable to assume that the cerium-hydrogen reaction is also rapid. Thus, the controlling step in the gettering process is assumed to be gas-phase mass transfer.

MODELS OF GAS-PHASE MASS TRANSFER

The diffusion of tritium in the gas phase to the surface of the particle can be expressed by the film theory of mass transfer, or by using a mass-transfer coefficient.

In the film-theory approach, diffusion is considered to occur across a thin film surrounding the solid pellet (Fig. 2). Flux through the film is given by^{76, *}

$$N_{Tr} = -0.1 c_{gas} D_{TA} \frac{dx_T}{dr} + x_T (N_{Tr}) \quad (1)$$

*For nomenclature definitions, see listing on page 33.

Fig. 2. Diagram illustrates film theory of mass transfer.

or

$$N_{Tr}(1-x_T) = -0.1 c_{gas}$$

$$D_{TA} \frac{dx_T}{dr} \quad (2)$$

Because $x_T \ll 1$ for this application,

$$\begin{aligned} N_{Tr} &\approx -0.1 c_{gas} D_{TA} \frac{dx_T}{dr} \\ &= -0.1 D_{TA} \frac{dc}{dr} \end{aligned} \quad (3)$$

The concentration gradient shown in Fig. 2 can be expressed as

$$\frac{dc}{dr} = -1000 \frac{(c - c_s)}{\delta} \quad (4)$$

which gives

$$N_{Tr} = + \frac{D_{TA}(c - c_s) \times 100}{\delta} \quad (5)$$

for the flux. Equation (5) gives the rate of gas-phase diffusion per unit surface area of getter, as described by the film theory of mass transfer. The mass-transfer coefficient, an empirical parameter, is used as follows:

$$N_{Tr} = 1000 k_x \frac{(c - c_s)}{c_{GAS}} \quad (6)$$

The mass-transfer coefficient k_x can be estimated for different physical situations, using existing empirical correlations. Both rates were applied to models of the process, thus providing a consistency check between the

two rate expressions. Comparing Eqs. (5) and (6) shows that

$$\frac{D_{TA}}{\delta} \times 0.1 = \frac{k_x}{c_{GAS}}, \quad (6a)$$

for the two models to be consistent.

Reactor Types Considered

Four types of reactors were considered for achieving the gas-solid contact necessary for gettinger:

- Fixed-bed reactor
- Moving-bed reactor
- Fluidized-bed reactor
- Cocurrent pneumatic-transport reactor.

The fixed-bed reactor is attractive because of its simplicity of design and construction and the relative ease with which it can be modeled. This type of reactor is discussed in detail in the following subsection. The moving-bed reactor is basically a fixed-bed reactor that can be continually replenished with new solids. This type of reactor is needed only if the solid is quickly de-activated or consumed. Since neither will be the case, moving beds are not considered further. The fluidized-bed reactor, suggested by Danner,⁷⁷ is attractive because of the greater gas-flow rate it can

handle. This type of reactor is also considered in greater detail later. The cocurrent pneumatic-transport reactor, in which the particles are blown along with the gas, is sometimes suitable for use with rapid chemical reactions.⁷⁸ However, because there are no established procedures for designing this type of reactor, it is not studied here.

Other reactor types considered briefly but not investigated in detail include packed fluidized beds, in which fluidization occurs in the interstices of large packings, and spouted beds, in which particles too large to fluidize flow upward in a fluid spout in the center of the bed and flow downward along the walls.

FIXED-BED REACTOR - MODELING AND RESULTS

A fixed-bed reactor (also called packed bed) consists of a vessel, usually cylindrical, with a batch of solid powder supported by a mesh screen or similar device (see Fig. 3). Gas flows downward through the

Fig. 3. Simplified diagram of fixed-bed reactor. In this type of reactor, gas flows downward through the vessel and the solid bed, providing very efficient gas-solid contact.

vessel and through the bed of solid getter particles. Gas-solid contact is very efficient in fixed-bed reactors.

The following formula can be derived to describe the performance of the fixed-bed reactor (see Appendix A):

$$\frac{dc}{dz'} = \frac{-A}{F} R. \quad (7)$$

The reaction rate R can be expressed in terms of the previously derived flux per unit surface area of particle N_{Tr} as follows:

$$R = aN_{Tr} \times 10^{-3}. \quad (8)$$

Combining Eqs. (5), (6), (7), and (8) gives

$$\frac{dc}{dz'} = \frac{-A}{F} \frac{aD_{TA}(c - c_s)}{\delta} \times 0.1, \quad (9)$$

for the film-theory mass-transfer model, and

$$\frac{dc}{dz'} = \frac{-A a k_x (c - c_s)}{F c_{gas}}, \quad (10)$$

for the mass-transfer-coefficient model.

The boundary condition for Eqs. (9) and (10) is at

$$z = 0, \quad c = c_o. \quad (11)$$

Now, integrating Eqs. (9) and (10) and applying Eq. (11), gives

$$c(z') = (c_o - c_s) \exp\left(\frac{-A}{F} \frac{aD_{TA}z}{\delta} \times 10^{-1}\right) + c_s \quad (12)$$

and

$$c(z) = (c_o - c_s) \exp\left(\frac{-A}{F} \frac{a k_x z}{c_{gas}}\right) + c_s. \quad (13)$$

The length of the mass-transfer zone L_{MTZ} and the volume of the mass-transfer zone V_{MTZ} (see Appendix A for explanation of mass-transfer zone) can be calculated using Eqs. (12) and (13). Using c_f for $c(z')$

in these equations means z' will equal L_{MTZ} and, solving for L_{MTZ} , gives

$$L_{MTZ} = \frac{F\delta}{AaD_{TA}} \times 10 \ln \left(\frac{c_o - c_s}{c_f - c_s} \right) \quad (14)$$

$$L_{MTZ} = \frac{Fc_{gas}}{Aak_x} \ln \left(\frac{c_o - c_s}{c_f - c_s} \right). \quad (15)$$

Solving for $V_{MTZ} = L_{MTZ} A$, gives

$$V_{MTZ} = \frac{F\delta}{aD_{TA}} \times 10^7 \ln \left(\frac{c_o - c_s}{c_f - c_s} \right) \quad (16)$$

$$V_{MTZ} = \frac{Fc_{GAS}^*}{ak_x} \times 10^6 \ln \left(\frac{c_o - c_s}{c_f - c_s} \right). \quad (17)$$

To design a bed for a specified set of conditions, the mass-transfer-zone volume is calculated using Eq. (16) or (17). Then, the additional volume needed to hold all the tritium to be fed to the bed is calculated as

$$V_{hold} = M_{T_2} / M \times 10^6. \quad (18)$$

Total bed volume is given by

$$V_{total} = V_{hold} + V_{MTZ}. \quad (19)$$

To apply Eqs. (14) through (19), values for the parameters c_o , c_s , M , F , δ , A , a , D_{TA} , c_{GAS} , and k_x must be calculated. These calculations are given in Appendix B and Appendix C (for k_x).

By comparing Eqs. (16) and (17), it is apparent that

$$\frac{\delta}{D_{TA}} = \frac{c_{GAS}}{k_x}, \quad (20)$$

which is simply the reciprocal of Eq. (6a).

To test the consistency of the film-theory and mass-transfer-coefficient correlations, a value of film thickness δ was calculated using Eq. (20) and checked against the expected value. For the parameter set $P = 101$ kPa, $T = 25^\circ\text{C}$, $\text{rad} = 0.150$ m, $D_p = 100$ μm , and $F = 10$ m³/s, Eq. (20) and the correlations in Appendices B and C give $\delta = 32$ μm . In fixed beds at low Reynolds numbers (for this bed, $\text{Re}' = 3.8$), δ typically approaches $D_p/2$. Thus, the film thickness would be expected to be about 50 μm , in reasonable agreement with the 32- μm calculated value. The mass-transfer-coefficient model was used here, since the two models for mass transfer appeared to be consistent. Parameters for the mass-transfer coefficient are more reliably estimated and the model more easily programmed on a computer.

To design a fixed-bed reactor - given the necessary parameters (c_o , c_f , F , rad , T , P , ϵ , D_p) - Eqs. (17), (18), and (19) give the volume and length of the bed. The pressure

drop across the bed must be calculated to see if it is reasonable (it should be as low as is practical).

To estimate bed pressure drop, the Ergun equation was used,

$$\left(\frac{\Delta P}{G^2}\right)\left(\frac{D_p}{L}\right)\left(\frac{\epsilon^3}{1-\epsilon}\right) = \left[\frac{150(1-\epsilon)}{(D_p G/\mu)}\right] \cdot 10^6 + 1.76. \quad (21)$$

For a bed with a significant pressure drop, gas density ρ decreases along the length of the bed. To account for this in using Eq. (21), the gas density at the end of the bed was calculated and then an average of the inlet and outlet densities was used to recalculate pressure drop. This procedure was then iterated until the average density converged to a single value.

To enable routine calculation of pressure drop and to allow consideration of many reactor configurations, three computer programs were written. Descriptions and listings of these programs and a sample output of each are contained in Appendix D.

Using the PACKEDBED2 program, reactor volume, length, and pressure drop were calculated for the following parameter values:

$$T = 25, 150, 250^\circ\text{C}$$

$$P = 101, 202, 505, 1010 \text{ kPa} \\ (1, 2, 5, 10 \text{ atm})$$

$$F = 1, 2, 5, 10 \text{ m}^3/\text{s}$$

(For F , flow through one bed, less than $10 \text{ m}^3/\text{s}$, several beds operated in parallel are required to achieve a system capacity of $10 \text{ m}^3/\text{s}$.)

$$D_p = 1, 10, 10^2, 10^3, 10^4 \text{ }\mu\text{m}$$

$$\epsilon = 0.3, 0.4$$

(True value for bed is unknown, variation was made to determine if value had significant effect.)

$$\text{rad} = 0.20, 0.40, 0.60, 0.80, 1.0 \text{ m.}$$

With the results from PACKEDBED2, the other programs were used to choose a prototype design for the fixed-bed reactor.

The following general observations can be made about the performance of packed beds:

- Increasing inlet pressure decreases required bed volume (although the effect is small)
- Increasing temperature decreases bed volume (also a small effect)
- Increasing void fraction has little effect on outlet tritium concentration, but decreases bed pressure drop

- Virtually all of the total bed volume is required as mass-transfer-zone volume; a few hundred cm^3 of cerium are sufficient to hold the tritium which has to be absorbed in the bed.

An imposed restraint in this study was minimizing getter material inventory to maximize (relatively) tritium concentration in the getter for easier recovery. Also, for large particles, the deep interior regions could not be used effectively while, for small particles, prohibitively large pressure drops were experienced. Thus, 100- μm -diam particles were chosen for the study. Even at this size, the pressure drop dictated the L/D ratio of the bed to be very small, $L/D \ll 1$.

In future studies, bed configuration could be optimized by applying the getter material onto an inert substrate. This would substantially reduce getter material inventory while achieving the larger particle sizes needed to obtain low pressure drops and L/D ratios of 5 to 10.

The prototype reactor design is shown in Fig. 4. The bed is indeed very shallow - about 20 mm deep. Such a bed could be constructed with suitable baffles to keep the getter particles from shifting.

The 20-mm bed depth is deeper than that needed for a 1% approach to equilibrium, which was the design criteria (see Appendix B). But, a much shallower depth, while able to reach a 1% approach, would mean a bed very difficult to construct and operate. A bed 20 mm thick, on the other hand, is much easier to build and yet still has a reasonable pressure drop of 20 kPa (3 psi). The large empty chamber above the bed serves to even out gas flow across the entire bed.

To save gas heating and pumping costs, the bed was designed to operate at room temperature and atmospheric pressure. A bed of somewhat smaller diameter and larger L/D would be possible at higher pressure, but the expense of a larger compressor would cancel any savings in reactor cost. As it is, circulating the gas will require a large blower. Incorporating the getter into a filter might be another way of achieving the desired solid-gas contact for a bed with this pancake shape.

FLUIDIZED-BED REACTOR - MODELING AND RESULTS

In a fluidized-bed reactor (Fig. 5), the solid getter particles are supported by the gas flowing upwards around them. The solids are dispersed by gas to form an "emulsion phase;" bubbles of gas flow upward through

Fig. 4. Prototype design for fixed-bed getter reactor.

Fig. 5. Simplified diagram of fluidized-bed reactor. Gas-solid contact is not as efficient in this type of reactor as in a fixed-bed reactor, but a much higher gas flow rate can be recommended.

the emulsion, carrying much of the gas flow in them. Because much of the gas flows through bubbles, which are not in intimate contact with the solids, the gas-solid contact is less efficient than in a packed bed, where the entire gas flow is in close contact with solids.

An attractive feature of fluidized beds, however, is the fact that once the bed is fluidized, increasing the gas-flow rate has essentially no effect on the pressure drop. This is in contrast to a packed bed, where increasing gas flow increases pressure drop sharply. In a fluidized bed, gas

velocity need only be low enough that the bed material is not blown out of the reactor. (See Ref. 78 for a more detailed description of fluidized-bed behavior.)

Development of successful models for fluidized beds has been hampered by the complexity of the fluidization phenomenon. No totally satisfactory model exists, though the literature is replete with suggested models.⁷⁹⁻¹⁰⁶ Most of these models require the use of parameters that can only be determined experimentally, and this was beyond the scope of this study. Two models not requiring experimental data are the bubble-assemblage model by Kato and Wen⁸⁸ and the fluid-bed model by Lanneau.¹⁰³ Of these, the bubble-assemblage model is the more theoretically sophisticated. Also, this model is designed for use with a computer, while the Lanneau model is not. For these reasons, the bubble-assemblage model was used in this study.

The bubble-assemblage model represents the fluidized bed as a series of compartments. The height of each compartment is equal to the bubble size at that location in the bed (bubbles grow in size as they travel up the bed due to bubble coalescence and decreasing pressure). Each compartment contains a bubble phase and an emulsion phase consisting of solid particles dispersed in gas.

Gas interchange occurs between the two phases. The reaction occurs in the emulsion phase, where solids are present.

The bubble-assemblage model is applicable only for beds that contain fairly small solid particles.⁸⁸ For particles larger than about 500 μm , the model gives meaningless results. A few needed parameters not given by Kato and Wen are given by Kunif and Levenspiel.⁷⁸

To predict the size of bubbles at the lower end of the fluidized bed, the type of flow distributor at the gas entrance to the bed must be specified. With a perforated-plate distributor, bubble size is a function of the number of perforations. Initially, the number of holes in the plate was set arbitrarily. In later studies, the number of holes was determined by specifying the radius of each hole in the plate and the fraction of plate surface to comprise the total perforation area.

The bubble-assemblage model, developed for a gas-solid catalytic reaction, uses a reaction rate of gas with solid. Models developed for noncatalytic reactions generally use the shrinking-core reaction model, in which the reactants diffuse through an ever-increasing layer of reacted solid.^{78,79} Since the solid-state diffusion step was not taken to be controlling in the gettering process,

the catalytic-reaction model, in which the reaction occurs on the particle surface, was used.

In a catalytic reaction, the solid is not consumed; whereas, strictly speaking, it is consumed in the gettering operation. However, we expect that the fluidized-bed reactor, like the fixed-bed reactor, will contain much more getter than is required to react with all the tritium. Therefore, the getter will be consumed only slightly and the catalytic-reaction model should be approximated reasonably well.

The bubble-assemblage model is most easily used for a first-order reaction: $R = kc \text{ kmol/m}^3\text{s}$. Combining Eqs. (5) and (8) gives

$$R = \frac{D_{TA} a (c - c_s)}{\delta} \times 10^{-1} \quad (22)$$

for the mass-transfer rate, which is assumed to be the reaction rate. For our purposes, $c_s \ll c$ so that the following approximation can be made:

$$R \approx \frac{D_{TA} a}{\delta} c \times 10^{-1} \quad (23)$$

By the definition of reaction-rate constant k , we get

$$k = \frac{D_{TA} a}{\delta} \times 10^{-1} \quad (24)$$

This form of rate constant k is used in the model. The corresponding

mass-transfer-coefficient rate expression was not used because a reliable correlation for k_x does not exist for fluidized beds. Three computer programs using the bubble-assemblage model are described in Appendix E, including sample data for each.

Using program FLUIDBED2, bed sizes were calculated for the following parameter values:

$$T = 25 \text{ and } 250^\circ\text{C}$$

$$P = 101, 505, 1010 \text{ kPa (1, 5, 10 atm)}$$

$$F = 1, 2, 5, 10 \text{ m}^3/\text{s}$$

(For F - flow through one bed - less than $10 \text{ m}^3/\text{s}$, several beds operated in parallel are required to achieve a system capacity of $10 \text{ m}^3/\text{s}$.)

$$D_p = 100 \text{ } \mu\text{m}$$

$$\text{Bed radius} = 0.50, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, 6.0 \text{ m}$$

$$\text{GWT} = 1, 5, 10, 50, 250, 500, 750, 1000 \text{ kg}$$

$$\delta = (D_p/2) \cdot (0.1, 1, 10)$$

(Since the actual value was unknown, the value in a fixed bed was assumed, and the sensitivity of design to this parameter was tested by varying by factors of 10.)

$$\epsilon_{mf} = 0.4, 0.5, 0.6$$

(Proper value is unknown; variation was made to determine sensitivity of results to this parameter.)

$$\text{Number of holes in perforated plate} = 10^2, 10^3, \text{ and } 10^4.$$

With the results from FLUIDBED2, the other programs were used to choose a prototype design for the fluidized-bed reactor.

In designing the prototype bed, performance was calculated for all combinations of δ and ϵ_{mf} given above, in that the proper values were not known. The prototype bed met the condition that, for all δ and ϵ_{mf} value combinations, the outlet concentration c_f was no larger than 10% of the inlet concentration c_o . A 10% residual concentration was used instead of the 1% used for the fixed bed, in recognition of the less efficient gas-solid contact in the fluidized bed.

Again, a few general observations can be made regarding the performance of fluidized beds. They are:

- Gas velocity in a fluidized bed is constrained to a certain region. With velocities too slow, the bed will not fluidize; with velocities too fast, the bed will blow out of the reactor. The

maximum velocity is equal to the terminal velocity a particle would attain while falling through a gas at the same conditions that exist in the reactor. For a 100- μm -diam particle of cerium in argon at atmospheric pressure and 25°C, the maximum velocity is about 1.29 m/s. The minimum fluidization velocity for these conditions is 0.0177 m/s.

- The minimum cross-sectional area of the reactor is determined by the total flow and the maximum velocity. For a $10\text{-m}^3/\text{s}$ flow at 1.29 m/s, the reactor area must be at least 7.75 m^2 , corresponding to a vessel $\sim 3.20\text{ m}$ in diameter. Thus, the fluidized bed must be about the same size as the fixed bed, or even larger. In practice, gas velocity must be considerably below maximum, requiring a vessel larger than indicated above.
- The fluidized bed must be fairly shallow (especially with a large-diameter bed) to have a reasonably small inventory of getter metal. Since a fluidized-bed reactor must be at least as large as a fixed-bed reactor, it should

also be about as shallow. But, if the fluidized bed is too shallow, the bubbles may not form in the bed before the gas reaches the top of the bed, resulting in poor fluidization.

- Bed performance is very sensitive to variations in ϵ_{mf} and δ . Increasing ϵ_{mf} decreases outlet concentration. Increasing δ increases outlet concentration, as expected.
- Increasing the number of perforations in the distribution plate effectively makes the gas bubbles smaller. For the prototype design, if more than about 2.0×10^5 holes are used, the bubbles become so small that this model is not applicable. Good design practice¹⁰⁷ suggests having the hole area equal to about 10% of the distributor plate area. Assuming 2.0×10^5 holes and a hole area of 10% gives a hole diameter of about 3.5 mm.
- The calculated pressure drop in the fluidized bed was quite small - about 0.5 kPa (0.07 psi). The perforated-plate pressure drop, estimated using correlations given by Perry,¹⁰⁷ was found to be

insignificantly small for the prototype bed.

The prototype fluidized-bed reactor is shown in Fig. 6. Two beds in parallel are required to attain a total flow of $10 \text{ m}^3/\text{s}$ and to satisfy the 10% residual criterion for all values of δ and ϵ_{mf} (at atmospheric pressure and 25°C). The beds are very shallow (about 30 mm deep) and are about 5 m in diameter. Such shallow beds will probably require internal baffles to keep the solids evenly distributed, despite the fluid nature of the bed. The large chamber below each bed serves to allow the gas to become uniform in pressure and velocity before entering the bed. The 6-m-high space above each bed is necessary for most of the particles to disengage from the gas and fall back to the bed surface.

It might be possible to use only one fluidized bed. But, experimental data or use of another model would be necessary to check this possibility.

COMPARISON OF FIXED- AND FLUIDIZED-BED REACTORS

Advantages of the fixed-bed reactor are:

- The fixed-bed reactor design is more reliable and likely to work as expected than the

fluidized-bed design. The art of fixed-bed modeling is more advanced than fluidized-bed modeling because the physical processes in the former are simpler and better understood.

- For a total flow of $10 \text{ m}^3/\text{s}$, the fixed-bed reactor contains only 650 kg of cerium, whereas the fluidized-bed reactor contains 2000 kg.
- One fixed-bed reactor 3.5 m in diameter can handle the entire $10\text{-m}^3/\text{s}$ flow, while two fluidized-bed reactors 5.0 m in diameter are required for the same flow.
- A fixed-bed reactor should be simpler to construct and operate than a fluidized-bed in that a fluidized-bed reactor requires more critical flow control to ensure proper bed fluidization.

Advantages of the fluidized-bed reactor are:

- Pressure drop in a fluidized-bed is very small - about 0.5 kPa (0.07 psi) - compared to 20 kPa (3 psi) in a fixed bed. Thus, gas pumping costs are less for a fluidized-bed reactor.

Fig. 6. Prototype design for fluidized-bed getter reactor.

- Because solids can be constantly removed from a fluidized bed, it is possible to replenish the bed continuously with fresh getter material, making continuous fluidized-bed operation feasible. A fixed-bed reactor, on the other hand, can only be operated in a batch mode.
- The continual replenishment of getter material in a fluidized bed makes it possible to maintain the getter in a relatively fresh state. (In a fixed bed, the getter becomes more and more tritided as the bed operates.) This getter freshness should mean more efficient fluidized-bed performance relative to a fixed-bed.
- The abrasive action of the solids against each other and the reactor walls in a fluidized bed may tend to scrub off the outer layer of tritided getter (or a layer of getter reacted with an impurity, such as oxygen). This will help maximize the getter reaction rate.
- A fluidized bed can be operated in a more flexible manner than a fixed bed. For example, in a fluidized

bed, gas velocity can be increased without significantly increasing bed pressure drop while, in a fixed-bed reactor, increasing gas velocity increases pressure drop sharply.

- Reactor design is somewhat uncertain due to the assumption that gas-phase mass transfer is the controlling step. If a different step were the controlling factor (i.e., one slower than gas-phase mass transfer), the size of the fluidized-bed reactor could be readily increased by adding more getter while retaining modest bed pressure drops. Increasing the amount of getter in a fixed bed, however, would quickly increase the bed pressure drop to excessive levels.

Continuing problems with fluidized-bed reactors include:

- Very thin beds may not fluidize properly. Experiments with different distributor-plate designs are needed.
- The abrasive effect of cerium on the reactor walls is not known.

Because of the small amount of tritium to be gettered, heat transfer in both types of beds should be sufficient to ensure isothermal operation (see Appendix F).

Considering the factors mentioned above, the fixed-bed reactor has more advantages than the fluidized-bed reactor and, as

presently modeled, the fixed-bed reactor is the more desirable of the two. However, if getter-reactor volume should need to be greatly expanded due to a different controlling step in the reaction model, the fluidized-bed reactor would be more adaptable because of its lower pressure drop.

Conceptual Design of Getter System

Conceptual designs were made of systems using the fixed- and fluidized-bed reactors to identify potential problems with the two concepts. These system designs are shown in Figs. 7 and 8, respectively. Details of the reactors are shown in Figs. 5 and 6, respectively. Each system can process $10 \text{ m}^3/\text{s}$ total flow at atmospheric pressure and 25°C . The fixed-bed system reduces the inlet tritium concentration by 100. The fluidized-bed system reduces it by 10. A summary of comparable fixed- and fluidized-bed parameters is given in Table 2.

By using multiple units, each of the systems can accommodate the much larger flows anticipated in CTR application. For example, multiple units are assumed in Figs. 7 and 8, where the use of blowers from another unit are suggested for blowing out the getter beds.

Each system contains the following components: gas blower, getter reactor(s), cyclone separator, getter regenerator and storage, and inter-connecting pipes and valves. In addition, two sets of gas-flow paths are shown in each diagram. The solid paths represent normal operation. The dashed paths represent operations to regenerate the tritided cerium getter.

FIXED-BED GETTER SYSTEM

In Fig. 7, the gas to be cleaned is compressed to the inlet pressure of the reactor and then passed downward through the reactor. A cyclone separator removes any particles that might have worked through the bed and supporting mesh. The cleaned gas is then returned to the atmosphere.

The getter is regenerated in a separate operation. First, the

Fig. 7. Conceptual design of fixed-bed getter system. Solids could be dispersed by rotating-disc sprayer or by perforated-pipe distributor. An auxiliary blower - perhaps from another unit - could be used to blow out the bed (would need total flow of about $15 \text{ m}^3/\text{s}$ to blow out one reactor).

getter material is removed from the bed by reversing flow through the reactor and using existing and/or auxiliary blowers to blow the material out the top of the reactor. The cyclone separator removes the solids and the flush gas is recirculated until the reactor is empty.

The getter is passed from the cyclone separator to a regenerator, where the tritide is decomposed and tritium is recovered. After getter regeneration, the bed is refilled using a particle-distributor mechanism. This mechanism could be a perforated tube through which the

Fig. 8. Conceptual design of fluidized-bed getter system. Solids could be dispersed by rotating-disc sprayer or by perforated-pipe distributor. An auxiliary blower - perhaps from another unit - could be used to blow out the bed (would need total flow of about $30 \text{ m}^3/\text{s}$ to blow out one reactor).

getter is blown, a spray device to spread the getter around, or some other device. If solids that come out of the bed during normal operation are regenerated immediately, they could be returned directly to the bed by the same distributor mechanism.

FLUIDIZED-BED GETTER SYSTEM

Figure 8 shows a similar system for a fluidized-bed reactor. The main differences between this and the

fixed-bed system are that the fluidized-bed system uses two reactors instead of one and the piping required to reverse gas flow to blow out the fixed bed is not necessary for getter regeneration in the fluidized bed. An auxiliary blower is needed, however, to blow the getter out of the fluidized bed; even if the entire $10\text{-m}^3/\text{s}$ flow is channeled through only one of the reactors, the velocity would not be sufficient to blow out the bed.

Table 2. Comparison of fixed- and fluidized-bed getter systems to treat $10 \text{ m}^3/\text{s}$ of argon contaminated with tritium.

	Fixed bed	Fluidized bed
Getter material	cerium powder	cerium powder
Getter particle diameter (μm)	100	100
Mass of getter in each bed (kg)	650	1000
Number of beds in system	1	2
Bed diameter (m)	3.5	5.0
Bed depth (mm)	20	40 (fluidized)
Height of bed vessel (m)	4.5	10-11
Ratio of outlet to inlet concentrations	0.01	0.1
Pressure drop across bed (kPa)	20	0.5

GETTER REGENERATION

To regenerate the getter, it must be heated so that the tritide-dissociation pressure permits tritium recovery. In the only experimental work reported, the tritide was melted to decompose it; cerium hydride melts at 1080°C , but a lower temperature probably would suffice. Operating a regeneration system at 1080°C will require the use of special materials (e.g., beryllium oxide, graphite, or refractory metals) and will require secondary containment of the regenerator. The regenerator will be operated at a very low pressure to permit T_2 recovery at the lowest temperature and/or fastest rate.

Three possible regenerator configurations that will melt the getter are shown in Figs. 9, 10, and 11. These configurations are presented in concept only, as specific designs are beyond the scope of this report. If melting the getter proves unnecessary, regeneration could be accomplished simply by heating the getter in a vessel connected to a suitable pump to remove the tritium released.

GETTER SYSTEM MODIFICATIONS

A possible refinement of the getter system would be to use two separate getter-bed systems, one to selectively remove impurities from the feed gas and the other to remove

Fig. 9. Semi-continuous regenerator concept. At 1100°C , CeTx particles melt, releasing T_2 . The molten Ce particles then agglomerate and fall rapidly to the bottom of the chamber.

Fig. 10. Batch-mode regenerator concept. Here, furnace chamber is filled with CeTx and heated to 1100°C, melting the CeTx and releasing T₂. The molten Ce is then allowed to cool and harden. Bottom of furnace is then opened so the solid Ce falls into the holding chamber from where it is eventually fed through a grinder back into the getter system.

Fig. 11. Continuous regenerator concept. In this system, spent getter is fed through a hopper onto a conveyor belt. As it moves along on the belt, it melts and releases T_2 . At the end of the furnace chamber, the molten Ce falls from the belt through a cooling chamber where it hardens back to solid form. It is then crushed to 100- μm -diam size and routed back into the getter system.

the tritium. Cerium reacts with oxygen, nitrogen, carbon monoxide, and carbon dioxide; system performance

might be improved by providing a separate bed to remove these impurities before scavenging the tritium.

Estimated System Capital Cost

Comparing the estimated capital cost of a getter system versus that of a catalytic-oxidation system further supports our interest in the getter approach. The cost figures used here are necessarily very rough because the system design itself is not well defined. Also, no attempt was made to optimize performance. Nonetheless, the getter approach definitely appears economically competitive with the traditional catalytic-oxidation technique. Cost figures for both types of getter system are given in Table 3. The cost of each item includes transportation and installation. Following are descriptions of the items used in computing these cost estimates:

- Blower - The blower must handle $10 \text{ m}^3/\text{s}$ at $\sim 100 \text{ kPa}$ ($\sim 1 \text{ atm}$) and 25°C . For the fixed-bed system, the blower must increase the pressure $\sim 20 \text{ kPa}$ ($\sim 0.2 \text{ atm}$). This requires a blower of some 300 to 370 kW (400 to 500 hp). The blower would probably be a multi-stage centrifugal compressor. The \$175,000 cost estimate agrees reasonably well with cost data given by Perry.¹⁰⁷ Since the pressure increase is less in a fluidized bed, the cost estimate is less: \$125,000.
- Reactor vessels - For the fixed bed, a cylindrical vessel 3.5 m in diameter and about 4.5 m tall is estimated to cost \$100,000. The same cost is assumed for each of the fluidized-bed reactor vessels (despite their larger size) for a total cost of \$200,000.
- Cyclone separators - Two separators operating in series are needed to clean the gas of fine dust particles. Each separator is estimated to cost \$50,000.
- Cerium - This getter material is available in kilogram quantities in powdered form at about 25¢/g and in ingots form at about 8.8¢/g.¹⁰⁸ The cost of inventory - 650 kg for a fixed-bed system and 2 Mg for a fluidized-bed system - is given for both prices. The price of cerium will probably drop when it is ordered in ton quantities, but this effect is not included in cost estimates here.

Table 3. Comparison of capital cost estimates for fixed- and fluidized-bed getter systems (with 10 m³/s capacity).

	Fixed bed	Fluidized bed
Blower	\$ 175,000	\$ 125,000
Reactor vessel(s)	100,000	200,000
Cyclone separators	100,000	100,000
Cerium inventory		
@ 25¢/g	163,000	500,000
@ 8.8¢/g	57,000	176,000
Instrumentation and computer controls	60,000	80,000
Piping and installation (pipes, valves, flanges, installation, and inspection)	240,000 210,000	240,000 210,000
Regeneration	200,000	200,000
Totals		
Ce @ 25¢/g	\$1,250,000	\$1,660,000
Ce @ 8.8¢/g	\$1,150,000	\$1,330,000

● Instrumentation and computer controls

- Here, the cost of instrumenting a large catalytic-oxidation system³ was pro-rated to a flow rate of 10 m³/s. The estimate was then increased for the fluidized-bed system to account for the more sophisticated controls required.

● Piping and installation

- About 75 m of 0.9-m (ID) pipe will be required, with about 12 valves and necessary flanges, at an estimated cost of \$240,000. An additional \$210,000 is allotted for installation and inspection.

● Regenerator unit

- This unit is estimated to cost \$200,000.

No contingency fee is shown in Table 3 because none is given for the catalytic-oxidation system, in that the system is part of an overall plant having an overall contingency factor. Thus, by not including a contingency fee in our estimates, the numbers are directly comparable. The final cost estimates are shown in Table 3.

From Table 3, we see that the fixed-bed system is less expensive than the fluidized-bed system, primarily due to the difference in

cerium inventory required. For cerium purchased as ingots instead of powder, the cost difference shrinks from \$410,000 to \$180,000. The fluidized-bed system is expected to be more expensive, since fluidization is a less efficient method of gas-solid contact than a fixed bed.

The capital cost of a getter system, based on a $1\text{-m}^3/\text{s}$ flow, is between $\$115,000/(\text{m}^3/\text{s})$ and $\$166,000/(\text{m}^3/\text{s})$, certainly competitive with a comparable catalytic-oxidation system costing an estimated $\$330,000/(\text{m}^3/\text{s})$.³

Conclusions and Recommendations

The major conclusion of this study is that it appears feasible to use chemical getters as tritium scavengers. Moreover, doing so could lead to a considerable reduction in capital cost compared to the large catalytic-oxidation systems now used. A summary of costs and important performance parameters for the two types of getter systems and the catalytic purification system is shown in Table 4.

All results reported here are for processes at 25°C and 101 kPa (1 atm). The getter concept, however, can be applied at higher temperatures and pressures, such as those found in a CTR helium-cooled blanket.

Cerium hydride has a sufficiently low partial pressure that cerium will perform quite well even at 200 to 250°C . And, high pressure should actually increase the system's gettering ability in that the partial pressure of tritium in the gas is increased. A getter system, therefore, could be used to recover tritium for CTR blankets.

Finally, based on the findings of this study, the following recommendations are made:

- The rate-controlling step of the gettering process must be determined. Suitable experiments to do this are

Table 4. Summary of costs and performance parameters for fixed- and fluidized-bed chemical getter systems and catalytic purification system to scavenge tritium from argon.

	Fixed bed	Fluidized bed	Catalytic purification
Capital cost, \$/(m ³ /s capacity)	115,000	133,000	330,000
Getter or adsorbent	Cerium	Cerium	Molecular sieve
Cerium inventory, kg/(m ³ /s capacity)	65	200	---
Operating temperature and pressure	Ambient*	Ambient*	Ambient*
Purification ratio, c_f/c_o	0.01	0.1	---
Design purification level, $\mu\text{Ci}/\text{m}^3$	500	<500	<500
Form of tritium when recovered	T ₂	T ₂	T ₂ O

*The effects of impurities on chemical getters is uncertain. Impurities do require elevated temperatures with catalytic purifiers.

- described in Refs. 109 and 110.
- The effect of poisoning on the gettering rate, if any, should be determined experimentally with cerium for anticipated impurities. The use of other getters, or the use of supplemental traps designed to pre-getter the impurities, should also be considered.
- Getter cost could be reduced if mischmetal could be used instead of pure cerium. Therefore, mischmetal should be studied for its hydrogen gettering ability.
- The dissociation pressure and decomposition rate of cerium hydride should be measured for an extended temperature range. It should be possible to reduce

regenerator temperature below 1100°C and thereby considerably reduce regeneration cost.

- Scale-model fixed and fluidized beds should be operated to verify the models used here. Parameters such

as bed-void fractions should be measured instead of estimated.

- Alternative reactor configurations (e.g., an entrained-bed reactor) should also be investigated.

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Nomenclature

a	Surface area of particle/volume of bed (m^2/m^3)
A	Cross-sectional area of bed (m^2)
B	Number of beds splitting total $10\text{-m}^3/\text{s}$ flow
c	Concentration of tritium in inert gas (mol/m^3)
c_f	Concentration of tritium in gas exiting reactor (mol/m^3)
c_{gas}	Total concentration of gas (mol/m^3)
c_o	Concentration of tritium in reactor feed gas (mol/m^3)
c_s	Concentration of tritium in gas in equilibrium with hydride getter (mol/m^3)
D	Diameter of bed (m)
D_p	Getter particle diameter (μm)
D_{TA}	Diffusion coefficient of tritium in argon (cm^2/s)
F	Volumetric flow of gas through bed (m^3/s)
G	Specific mass velocity in bed ($\text{kg}/\text{m}^2 \text{ s}$)
GWT	Weight of getter in fluidized bed (kg)
HOLES	Number of perforations in fluidized-bed distributor plate (unitless)
j_D	J-factor for mass transfer (unitless)
j_H	J-factor for heat transfer (unitless)
k	First-order reaction-rate constant ($\text{kmol}/\text{mol s}$)
k_x	Mass-transfer coefficient ($\text{kmol}/\text{m}^2 \text{ s}$)
L	Length of bed (mm)
L_{MTZ}	Length of mass-transfer zone (mm)
M	Capacity of bed for tritium ($\text{kmol T}_2/\text{m}^3 \text{ bed}$)
M_{T_2}	Total amount of tritium to be fed to bed (mole)
N_{Tr}	Tritium flux in radial direction ($\text{mol}/\text{m}^2 \text{ s}$)

P	Gas pressure (kPa)
PHR	Radius of perforations in fluidized-bed distributor plate (mm)
PVF	Void fraction of fluidized-bed distributor plate (unitless)
r	Radial coordinate (mm)
R	Rate of hydrogen uptake per unit volume of bed ($\text{kmol/m}^3 \text{ s}$)
rad	Radius of getter bed (m)
Re	Reynolds number = $DV\rho/\mu$ (unitless)
Re	Modified Reynolds number = $G/a\mu$ (unitless)
Sc	Schmidt number = $\mu/\rho D_{TA} \times 10^4$ (unitless)
Sh	Sherwood number = $k_x D \times 10^7 / c_{\text{gas}} D_{TA}$ (unitless)
t	Duration of bed use (s)
u	Velocity of gas in fluidized bed (m/s)
u_{mf}	Minimum fluidization velocity of fluidized bed (m/s)
u_T	Maximum allowable velocity in fluidized bed (m/s)
V	Velocity of gas in reactor (m/s)
V_{HOLD}	Volume of bed needed to contain all tritium fed to bed (mm^3)
V_{MTZ}	Volume of mass-transfer zone (mm^3)
V_{TOTAL}	Total volume of bed (mm^3)
x_T	Mole fraction of tritium in gas (unitless)
z	Coordinate along length of bed, origin at front of bed (mm)
z'	Coordinate along length of bed, origin at front of unused portion of bed (mm)
δ	Gas film thickness across which diffusion occurs (μm)
ϵ	Void fraction of bed (unitless)
ϵ_{mf}	Void fraction of fluidized bed at minimum fluidization conditions (unitless)
μ	Viscosity of gas (kg/m s)
ρ	Gas density (kg/m^3)

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Appendix A: Derivation of Model for Fixed-Bed Reactor

A fixed-bed reactor can be modeled by writing a mass balance over a differential volume element of the reactor. A fixed bed is shown schematically in Fig. A-1. The concentration profile of tritium in the bed is shown in Fig. A-2. The shape of the concentration front remains the same - the front proceeds along the bed as more is added. The mass-transfer zone indicated in Fig. A-2 is the section of bed in which tritium is being removed. Getter material ahead of the mass-transfer zone is completely tritided, so no tritium is absorbed. At the end of the mass-transfer zone, the tritium level has been reduced to the minimum possible with the getter and no further mass-transfer occurs.

When the end of the mass-transfer zone reaches the end of the bed, "breakthrough" occurs and for practical purposes, the bed is saturated with tritium and of no further use without regeneration.

A mass balance can be written on a differential volume element in the mass transfer zone. To do this, a moving coordinate z' , with its origin at the beginning of the mass-transfer zone, is defined:

$$z' = z - \frac{F_c t}{A M} \quad (A-1)$$

In the moving-coordinate system, the mass balance is time independent, and becomes (considering only convective transport, and neglecting axial diffusion):

$$\frac{\text{Moles of } T_2 \text{ flowing into volume}}{\text{Unit time}} - \frac{\text{Moles of } T_2 \text{ flowing out of volume}}{\text{Unit time}} = \frac{\text{Moles of } T_2 \text{ removed}}{\text{Unit time}}$$

$$F_c \Big|_{z'} - F_c \Big|_{z' + \Delta z'} = R \Delta z' A. \quad (A-2)$$

Rearranging and taking the limit as $\Delta z' \rightarrow 0$ gives

$$\frac{dc}{dz'} = - \frac{A}{F} R. \quad (A-3)$$

Fig. A-1. Schematic of fixed getter bed.

Fig. A-2. Tritium-concentration profile for fixed getter bed.

Appendix B: Calculation of Parameters for Reactor Models

Parameter

Calculation

c_o

Initial concentration of T_2 is 3.8 ppm

$$\frac{3.8 \times 10^{-6} \text{ mol } T_2}{\text{mol Argon}} \times \frac{P \text{ (kPa)}}{\left(8.28 \times 10^3 \frac{\text{kPa (cm}^3\text{)}}{\text{mol K}}\right) (T \text{ K})} =$$

$$4.63 \times 10^{-10} \frac{P}{T} \frac{\text{mol}}{\text{cm}^3}$$

or

$$c_o = 4.63 \times 10^{-4} \frac{P}{T} \frac{\text{mol}}{\text{m}^3} \quad (\text{B-1})$$

c_s

$$\log_{10} P_{\text{torr}} = 10.72 - 10,840/T$$

$$c_s = \frac{(P_{\text{torr}})}{RT} = \frac{10^{(10.72 - 10,840/T)} \text{ torr}}{\left(82.057 \frac{\text{cc-atm}}{\text{mol K}}\right) T} \times \frac{1 \text{ atm}}{760 \text{ torr}}$$

or

$$c_s = \frac{10^{(10.72 - 10,840/T)}}{62,363 T} \times 10^6 \frac{\text{mol}}{\text{m}^3} \quad (\text{B-2})$$

c_{gas}

$$c_{\text{gas}} = P/RT = \frac{P \text{ (kPa)}}{\left(8.21 \times 10^3 \frac{\text{kPa (cm}^3\text{)}}{\text{mol K}}\right) (T \text{ K})}$$

or

$$c_{\text{gas}} = 1.22 \times 10^{-4} \frac{P}{T} \frac{\text{mol}}{\text{m}^3} \quad (\text{B-3})$$

ParameterCalculation ρ Gas density = concentration $\times$ molecular weight.

$$\therefore \rho = c_{\text{gas}} \times 40 \text{ or } \rho = 4.88 \times 10^{-6} \frac{\text{P kg}}{\text{T m}^3} . \quad (\text{B-5})$$

 F

Total flow through system is $10 \text{ m}^3/\text{s}$ at atmospheric pressure.
So, for inlet pressure P , with the flow split among B beds,

$$F = \frac{10}{B} \left(\frac{101}{P} \right) \frac{\text{m}^3}{\text{s}} . \quad (\text{B-5})$$

 δ

Typically, for a low-Reynolds-number fixed bed,

$$\delta = D_p / 2 \text{ cm} . \quad (\text{B-6})$$

 A

$$A = \pi(\text{rad})^2 \text{ m}^2 . \quad (\text{B-7})$$

 a For spherical particles packed with void fraction ϵ ,

$$a = \frac{6(1 - \epsilon)}{D_p} \times 10^6 \text{ m}^{-1} . \quad (\text{B-8})$$

 D_{TA} Using the Slattery and Bird equation for diffusivity,¹¹¹

$$D = (2.74 \times 10^{-4} / P) [M_1 + M_2] / M_1 M_2^{1/2} [P_{c1} P_{c2}]^{1/3} \\ (T_{c1} T_{c2})^{-0.495} T^{1.823} ,$$

ParameterCalculation

D_{TA}
(cont.)

where

$P [=]$ atm

$P_{c1}, P_{c2} [=]$ atm = critical pressure

$T_{c1}, T_{c2} [=]$ K = critical temperature

$T [=]$ K

$D [=]$ cm²/s.

For argon and tritium:

	M	T_c K	P_c atm
Argon	40	151.0 ¹¹¹	48.0 ¹¹¹
Tritium	6	43.7 ¹¹²	20.8 ¹¹²

$$D = 1.524 \times 10^{-5} \frac{T}{P}^{1.823} \frac{\text{cm}^2}{\text{s}} \quad P [=] \text{ atm}$$

$$D_{TA} = 1.544 \times 10^{-2} \frac{T}{P}^{1.823} \frac{\text{cm}^2}{\text{s}} \quad P [=] \text{ kPa.} \quad (\text{B-9})$$

M

Capacity of bed for tritium (k mol T₂/m³ bed). Bed capacity depends on the allowable concentration of tritium in the cerium getter. The pressure plateau for cerium hydride goes up to CeH₂. Therefore, theoretically 1 mole of hydrogen or tritium could be absorbed by 1 mole of cerium. However, tritides usually exhibit a higher dissociation pressure than hydride and, as the hydride approaches CeH₂, the actual pressure might well be higher than the equilibrium pressure. So, to be conservative, the tritide CeH_{0.5}³ is assumed to represent the fully utilized getter.

ParameterCalculation

M
(cont.)

For bed of 1 m³ volume, the volume of cerium is
(1 - ε) m³. The capacity of the bed for tritium, therefore,
is

$$\text{Capacity} = \left((1 - \epsilon) \text{ m}^3 \text{ Ce} \right) \left(\frac{6.7 \text{ g Ce}}{\text{cm}^3 \text{ Ce}} \right) \left(\frac{1 \text{ mol Ce}}{140 \text{ g Ce}} \right) \left(\frac{0.5 \text{ g atom T}}{\text{mol Ce}} \right)$$

$$\left(\frac{10^6 \text{ cm}^3}{\text{m}^3} \right) \left(\frac{1 \text{ mol T}_2}{2 \text{ g-atom T}} \right) = 0.0120(1-\epsilon) \frac{\text{mol T}_2}{\text{bed}}$$

(B-10)

M = capacity/unit volume of bed becomes

$$M = 1.20 \times 10^{-2} (1 - \epsilon) \frac{\text{mol T}_2}{\text{m}^3 \text{ bed}} = 1.2 \times 10^{-5} (1 - \epsilon) \frac{\text{k mol T}_2}{\text{m}^3 \text{ bed}}$$

(B-11)

Gas viscosity is estimated by using Eqs. 9 through 15 of
Reid and Sherwood.¹¹¹ For argon, this gives

$$\mu = 6.44 \times 10^{-3} (0.0303 T - 1.67)^{5/8} \text{ cp}$$

or

$$\mu = 6.44 \times 10^{-5} (0.0303 T - 1.67)^{5/8} \text{ g/cm s}$$

$$\mu = 6.44 \times 10^{-6} (0.0303 T - 1.67)^{5/8} \text{ kg/m s.}$$

Appendix C: Calculation of Mass-Transfer Coefficient for Fixed-Bed Reactor

Using J-factor correlations, the mass-transfer coefficient can be estimated for fixed-bed reactor⁷⁶ as follows:

$$j_D = Sh Re^{-1} S_c^{-1/3} \quad (C-1)$$

or

$$j_D = \frac{k_x}{c_{gas} V} \left(\frac{\mu}{\rho D_{TA}} \right)^{2/3} \cdot 10^{17/3} \quad (C-2)$$

By the analogy between heat and mass transfer,⁷⁶

$$j_d = j_H \quad (C-3)$$

For packed beds (fixed beds), the following empirical correlation has been developed:⁷⁶

$$j_H = 0.91 Re^{-0.51} \psi \quad (Re < 50) \quad (C-4)$$

$$j_H = 0.61 Re^{-0.41} \psi \quad (Re > 50) \quad (C-5)$$

where

$$Re = \frac{G}{a\mu} \quad (C-6)$$

and ψ is an empirical particle shape coefficient (for spherical particle, $\psi = 1$);⁷⁶

$$\therefore Re = G/a\mu \quad (C-7)$$

To obtain k_x , Re is first calculated using Eq. (C-7). Then, j_D is calculated using Eq. (C-4) or (C-5). Finally, k_x is calculated using Eq. (C-2).

Appendix D: Computer Program for Fixed-Bed Modeling

PROGRAM PACKEDBED1

This program calculates the volume of a reactor needed to achieve a 1% approach to equilibrium, that is

$$\left(\frac{c_f - c_s}{c_o - c_s} \right) = 0.01. \quad (D-1)$$

This approach to equilibrium was chosen as one typically exhibited by fixed-bed reactors with optimized designs. Combining Eq. (D-1) with Eqs. (17), (18), (19), and (C-2), (C-4), (C-5), and (C-7), the bed volume can be calculated. Applying Eq. (21) gives the bed pressure drop.

A listing (Table D-1) and an example of compiling and executing PACKEDBED1 (Table D-2) are provided to illustrate the following description:

PACKEDBED1 has teletype I/O. Upon compiling and executing the controllee, five pieces of data are requested by the program: T,P,M (the number of beds through which the total flow is to be split), DP (getter particle diameter), and EPS (bed-void fraction). Each number is entered in F10.2 format. These numbers are used throughout program execution; to change them, the program must be terminated and restarted. Temperature is in °C, pressure in atmosphere, particle diameter in μm . The program then requests bed radius in cm (also entered in F10.2 format).

If the specified radius is so small that the bed pressure drop is larger than the inlet pressure, a message to that effect is printed, and a new bed radius is requested. If the bed pressure drop is very close to the inlet pressure, the algorithm may not converge. If this occurs, the message "AFTER 500 LOOPS IT HAS NOT CONVERGED" will be printed, followed by five lines of numbers. If convergence is not attained after 500 loops, a new guess of density is made, and the algorithm restarted. If another 500 iterations do not give convergence, a message identical to the first is printed, followed by five lines of numbers and a request for a new bed radius. At this point, no further attempts are made to solve the specified problem. To determine what numbers are printed out, see lines 89 and 90 of the program listing.

If the algorithm converges, the bed length, radius, cross-sectional area, and volume are printed, as well as the inlet pressure and pressure drop. The bed dimensions give the minimum length for the specified bed radius to achieve a 1% approach to equilibrium; a longer bed will give a closer approach to equilibrium.

Entering zero for any parameter but T stops the program.

PROGRAM PACKEDBED2

This program uses the same set of equations as PACKEDBED1, but carries out the calculations described for PACKEDBED1 for all combinations of the following parameters:

T = 25, 150, 250°C

P = 101, 202, 505, 1010 kPa (k, 2, 5, 10 atm)

Number of beds = 1, 2, 5, 10

$D_p = 1, 10, 10^2, 10^3, 10^4 \mu\text{m}$

$\epsilon = 0.3, 0.4$

rad = 0.20, 0.40, 0.60, 0.80, 1.00 m.

Program output is directed to a high-speed printer. Table D-3 contains the listing of this program, followed by an example of the program being compiled and executed by teletype in Table D-4. Before execution starts, the message "RUN?" is printed. If execution is desired, a "1" is entered; if not, any other digit is entered. No other teletype output is produced until the program finishes.

One page of high-speed-printer output is shown in Table D-5 - 48 such pages are generated. The column headings have the same meaning as the same symbols in PACKEDBED1: T = temperature, °C; P = pressure, atm; M = number of beds; D_p = particle diameter, μm ; EPS = bed-void fraction; RAD = bed radius, cm; A = bed cross-sectional area, cm^2 ; L = bed length, cm; VOL = bed volume, cm^3 ; DELP = pressure drop across bed. If DELP is negative and, in absolute value, larger than P, the pressure drop across the bed was larger than the inlet pressure. If DELP is negative and, in absolute value, smaller than P, the algorithm did not converge.

Table D-1. PACKBED1 program listing.

```

1 PROGRAM PACKEDBED1(TAPE59)
2 REAL M,MU,JD,KX
3 CALL CHANGE(4R+PRG)
4 C ENTER PARAMETERS
5 T=M-P-DP*EPS=RAD=0.0
6 WRITE(59,"(" T")")
7 READ(59,1)T
8 I FORMAT(F10.2)
9 T=T+273
10 WRITE(59,"(" P")")
11 READ(59,1)P
12 WRITE(59,"(" M")")
13 READ(59,1)M
14 WRITE(59,"(" DP")")
15 READ(59,1)DP
16 DP=DP+1.0E-4
17 WRITE(59,"(" EPS")")
18 READ(59,1)EPS
19 IF(P.EQ.0.0.OR.DP.EQ.0.0.OR.M.EQ.0.0.OR.EPS.EQ.0.0)CALL EXIT
20 C CALCULATE CONSTANTS
21 CO=4.63E-8*P/T
22 CS=(10.+(10.72-10840./T))/(62363.*T)
23 MU=17.78E-5*((4.58+T/151.-1.67)**0.625)+1.0E-2/0.02763
24 AA=6.0*(1.0-EPS)/DP
25 TEMP1=760.*P=ALOG(100.)/(62363.*AA*T)
26 VOLC=3.6/(M*0.03445*EPS)
27 RHO1=P*40.*454./((1.314*T*((2.54*12.))**3))
28 C1=RHO1/40.
29 F1=1.0E7/(M*P)
30 DAB1=1.524E-5*(T**1.23)/P
31 ZERO=0.0
32 C START LOOP FOR SPECIFIC BED RADIUS
33 C 100 WRITE(59,"(/////" ENTER BED RADIUS, CM")")
34 READ(59,1)RAD
35 RAD=RAD+ZERO
36 IF(RAD.EQ.0.0)CALL EXIT
37 I=0
38 J=0
39 A=3.141592654*RAD*RAD
40 RHO1B=RHO1
41 C1B=C1
42 F1B=F1
43 V1B=F1B/A
44 DAB1B=DAB1
45 GO=17845.0/(M*A)
46 RE=GO/(AA*MU)
47 IF(RE.LE.50.0)GO TO 101
48 JD=0.61*(RE*(-0.41))
49 GO TO 102
50 JD=0.91*(RE*(-0.51))
51 CONTINUE
52 101 TEMP2=((150.+(1.0-EPS)/(DP*GO/MU))+1.75)*(1.0-EPS)*GO/GO/8
53 KX=JD*V1B*C1B*((DAB1B*RHO1B/MU)**(2.0/3.0))
54 I=1
55 VMTZ=TEMP1+F1B/KX
56 VOL=VMTZ+VOLC
57 L=VOL/A
58
59
60

```

Table D-1. (Continued)

```

61 DELP=TEMP2*L/RHO1B
62 IF(DELP.LE.P)GO TO 104
63 WRITE(59,8
64 "(/"" PRESSURE DROP IS LARGER THAN INPUT PRESSURE""")
65 GO TO 100
66 104 RHO2B=RHO1*(2.0*P-DELP)/(2.0*P)
67 F2B=F1*(2.0*P-DELP)/(2.0*(P-DELP))
68 V2B=F2B/A
69 DAS2B=DAB1*(2.0*P-DELP)/(2.0*(P-DELP))
70 IF(1.GT.500)GO TO 150
71 IF(ABS((V1B-V2B)/V1B).GT.1.0E-2)GO TO 115
72 IF(ABS((RHO1B-RHO2B)/RHO1B).GT.1.0E-2)GO TO 115
73 IF(ABS((DAB1B-DAB2B)/DAB1B).LE.1.0E-2)GO TO 120
74 115 V1B=V2B
75 F1B=F2B
76 DAB1B=DAB2B
77 RHO1B=RHO2B
78 C1B=RHO1B/40.
79 GO TO 105
80 120 WRITE(59,"(/"" BED DIMENSIONS""")
81 WRITE(59,"("" LENGTH,CM"" 10X,F10.4)""L
82 WRITE(59,"("" RADIUS, CM"" 9X,F10.4)""RAD
83 WRITE(59,"("" AREA, CM*CM"" 9X,F10.4)""A
84 WRITE(59,"("" VOLUME,CC"" 9X,F10.4)""VOL
85 WRITE(59,"(/"" BED INLET PRESSURE, ATM"" 7X,F10.4)""P
86 WRITE(59,"("" BED PRESSURE DROP, ATM"" 9X,F10.4)""DELP
87 GO TO 100
88 150 WRITE(59,"(/"" AFTER 500 LODPS, IT HAS NOT CONVERGED""")
89 WRITE(59,"(4E12.4)""RAD,A,RHO1B,RHO2B,C1B,F1B,F2B,8
90 V1B,V2B,DAB1B,DAB2B,GO,RE,JD,TEMP2,KX,VMTZ,VOL,L,DELP
91 IF(J.EQ.1)GO TO 100
92 J=1
93 RHO1B=(RHO1B+RHO2B)/2.0
94 C1B=RHO1B/40.0
95 V1B=(V1B+V2B)/2.0
96 F1B=(F1B+F2B)/2.0
97 DAB1B=(DAB1B+DAB2B)/2.0
98 I=0
99 GO TO 105
100 END

```

Table D-2. PACKBED1 compilation and execution.

Compile and create controllee

```
CHAT PACKEDBED1 PIGO PIBIN PILIST Y02 M M / 1 1.4
LOADING
CODE BLOC          PIGO WRITTEN
FILE SIZE=        0013527
FLD LGTH=         0013277   0011272
```

Execute controllee

```
PIGO / 1 1
T
25.0
P
1.0
M
1.0
DP
100.0
EPS
0.4
```

```
ENTER BED RADIUS, CM
200.0
```

```
BED DIMENSIONS
LENGTH, CM          0.0100
RADIUS, CM          200.0000
AREA, CM*CM         *.
VOLUME, CC          1261.9913
```

```
BED INLET PRESSURE, ATM      1.0000
BED PRESSURE DROP, ATM      0.0018
```

```
ENTER BED RADIUS, CM
150.0
```

```
BED DIMENSIONS
LENGTH, CM          0.0144
RADIUS, CM          150.0000
AREA, CM*CM         70685.8347
VOLUME, CC          1016.1364
```

```
BED INLET PRESSURE, ATM      1.0000
BED PRESSURE DROP, ATM      0.0050
```

```
ENTER BED RADIUS, CM
0,0 ENTER 0 TO END PROGRAM
```

ALL DONE

Table D-3. PACKBED2 listing.

```

1  PROGRAM PACKEDBED2(HSP)
2  REAL M,L
3  CALL CHANGE(4R+ABC)
4  L=A-VOL=DELP=0.0
5  IRUNC=0
6  WRITE(59,"( " RUN?" ")")
7  READ(59,"(1)")IRUNC
8  IF(IRUNC.NE.1)CALL EXIT
9  DO 1 IT=1,11,5
10 T=25.0+IT
11 IF(IT.EQ.11)T=T-25.0
12 DO 1 IP=1,4
13 P=IP
14 IF(IP.GE.3)P=IP+5.0-10.0
15 DO 1 IM=1,4
16 M=IM
17 IF(IM.GE.3)M=M+5.0-10.0
18 WRITE(3,100)
19 100 FORMAT("1" 7X,"T",8X,"P",9X,"M",7X,"DP",6X,"EPS",6X,&
20 "RAD",5X,"A",6X,"L",7X,"VOL",5X,"DELP"/)
21 DO 2 DP=1,5
22 DP=10.0*(DP-1)
23 DO 2 EPS=3,4
24 EPS=1EPS*0.1
25 DO 2 IRAD=20,100,20
26 RAD=IRAD
27 CALL DELP1(T,P,M,DP,EPS,RAD,L,DELP)
28 A=RAD+RAD*3.141592654
29 VOL=L*A
30 2 WRITE(3,101)T,P,M,DP,EPS,RAD,A,L,VOL,DELP
31 101 FORMAT(1X,2F9.1,2F9.0,2F9.2,2F9.1,F9.4,F9.1,F9.4)
32 1 CONTINUE
33 CALL EXIT
34 END

```


Table D-3. (Continued)

```

1  SUBROUTINE DELP1(T1,P,M,DP1,EPS,RAD,L,DELP)
2  REAL M,MU,JD,KX,L
3
4  C
5  C
6  CALCULATE CONSTANTS
7  T=T1+273.
8  DP=DP1*1.0E-4
9  CO=4.63E-8*P/T
10 CS=(10.**((10.72-10840./T)))/(62363.*T)
11 MU=17.76E-5*((4.58*T/151.-1.67)**0.625)*1.0E-2/0.02763
12 AA=6.0*(1.0-EPS)/DP
13 TEMP1=760.*P*ALOG(100.)/(62363.*AA*T)
14 VOLC=3.6/(M*0.03445*EPS)
15 RHO1=P*40.*454./((1.314*T*((2.54+12.))**3))
16 C1=RHO1/40.
17 F1=1.0E7/(M*P)
18 DAB1=1.824E-5*(T**1.623)/P
19 ZERO=0.0
20 C
21 C
22 START LOOP FOR SPECIFIC BED RADIUS
23 I=0
24 J=0
25 A=3.141592654*RAD*RAD
26 RHO1B=RHO1
27 C1B=C1
28 F1B=F1
29 V1B=F1B/A
30 DAB1B=DAB1
31 GO=17845.0/(M*A)
32 RE=GO/(AA*MU)
33 IF (RE.LE.50.0) GO TO 101
34 JD=0.61*(RE**(-0.41))
35 GO TO 102
36 JD=0.91*(RE**(-0.51))
37 CONTINUE
38 TEMP2=((150.*(1.0-EPS)/(DP*GO/MU)+1.75)*(1.0-EPS)*GO/GO)
39 (DP*EPS**3))*((1.4504E-5/14.7)
40 KX=JD*V1B*C1B*((DAB1B=RHO1B/MU)**(2.0/3.0))
41 I=I+1
42 VMTZ=TEMP1*F1B/KX
43 VOL=VMTZ+VOLC
44 L=VOL/A
45 DELP=TEMP2*L/RHO1B
46 IF (DELP.GE.P) GO TO 160
47 RHO2B=RHO1*(2.0*P-DELP)/(2.0*P)
48 F2B=F1*(2.0*P-DELP)/(2.0*(P-DELP))
49 V2B=F2B/A
50 DAB2B=DAB1*(2.0*P-DELP)/(2.0*(P-DELP))
51 IF (I.GT.100) GO TO 150
52 IF (ABS((V1B-V2B)/V1B).GT.1.0E-2) GO TO 115
53 IF (ABS((RHO1B-RHO2B)/RHO1B).GT.1.0E-2) GO TO 115
54 IF (ABS((DAB1B-DAB2B)/DAB1B).LE.1.0E-2) RETURN
55 V1B=V2B
56 F1B=F2B
57 DAB1B=DAB2B
58 RHO1B=RHO2B
59 C1B=RHO1B/40.
60 GO TO 105
61 IF (J.EQ.1) GO TO 160
62 J=J+1
63 RHO1B=(RHO1B+RHO2B)/2.0
64 C1B=RHO1B/40.0
65 V1B=(V1B+V2B)/2.0
66 F1B=(F1B+F2B)/2.0
67 DAB1B=(DAB1B+DAB2B)/2.0
68 GO TO 105
69 DELP=DELP
70 R=TURN
71 END

```

Table D-4. PACKBED2 compilation and execution.

Compile, create, and execute controllee

```
CHAT PACKEDBED2 P2GOS P2BIN P2LIST Y02 M M / 1 1.4
LOADING
CODE BLOC          P2GO WRITTEN
FILE SIZE=        0013442
FLD LGTH=         0013212    0011205
EXECUTION
RUN?
1
ALL DONE
```

Table D-5. Sample page of high-speed-printer output.

	1	T	P	M	DP	EPS	RAD	A	L	VOL	DELP
	1	1	1	1	1	0.30	20.0	1256.6	0.0799	100.4	*
						0.30	40.0	5026.5	0.0201	100.9	-526.6652
						0.30	60.0	11309.7	0.0090	101.3	-104.1629
						0.30	80.0	20106.2	0.0051	101.7	-33.0602
						0.30	100.0	31415.9	0.0033	102.1	-13.5905
						0.40	20.0	1256.6	0.0800	100.6	*
						0.40	40.0	5026.5	0.0201	101.1	-163.7491
						0.40	60.0	11309.7	0.0090	101.6	-32.4053
						0.40	80.0	20106.2	0.0051	102.2	-10.2943
						0.40	100.0	31415.9	0.0033	102.7	-4.2359
					10	0.30	20.0	1256.6	0.0909	114.2	-114.9229
					10	0.30	40.0	5026.5	0.0255	128.0	-6.9977
					10	0.30	60.0	11309.7	0.0125	141.6	-1.4871
					10	0.30	80.0	20106.2	0.0075	150.0	0.8891
					10	0.30	100.0	31415.9	0.0057	178.0	0.2754
					10	0.40	20.0	1256.6	0.0938	117.9	-37.8482
					10	0.40	40.0	5026.5	0.0269	135.3	-2.3123
					10	0.40	60.0	11309.7	0.0133	150.5	0.6731
					10	0.40	80.0	20106.2	0.0088	176.6	0.2001
					10	0.40	100.0	31415.9	0.0060	190.1	0.0823
					100	0.30	20.0	1256.6	0.4447	558.9	-14.4495
					100	0.30	40.0	5026.5	0.2234	1122.8	-1.4820
					100	0.30	60.0	11309.7	0.1412	1597.2	0.2272
					100	0.30	80.0	20106.2	0.0969	1947.7	0.0741
					100	0.30	100.0	31415.9	0.0751	2359.0	0.0346
					100	0.40	20.0	1256.6	0.5404	679.1	-6.0579
					100	0.40	40.0	5026.5	0.3018	1517.1	0.5769
					100	0.40	60.0	11309.7	0.1647	1862.2	0.0783
					100	0.40	80.0	20106.2	0.1186	2384.1	0.0281
					100	0.40	100.0	31415.9	0.0924	2903.9	0.0131
					1000	0.30	20.0	1256.6	10.0392	12615.7	-23.1823
					1000	0.30	40.0	5026.5	4.2055	21139.1	-1.2859
					1000	0.30	60.0	11309.7	4.2044	47550.2	0.1788
					1000	0.30	80.0	20106.2	2.9412	59137.1	0.0455
					1000	0.30	100.0	31415.9	2.9915	71991.1	0.0177
					1000	0.40	20.0	1256.6	12.4573	15654.3	-10.3348
					1000	0.40	40.0	5026.5	6.1785	41109.6	0.7721
					1000	0.40	60.0	11309.7	5.0325	56916.8	0.0699
					1000	0.40	80.0	20106.2	3.6313	73011.0	0.0187
					1000	0.40	100.0	31415.9	2.8913	90832.9	0.0074
					10000	0.30	20.0	1256.6	256.0823	321802.8	-56.7269
					10000	0.30	40.0	5026.5	145.0306	729003.2	-2.0363
					10000	0.30	60.0	11309.7	126.88681	435056.3	0.4675
					10000	0.30	80.0	20106.2	85.30541	715166.4	0.0822
					10000	0.30	100.0	31415.9	69.33552	178238.3	0.0277
					10000	0.40	20.0	1256.6	318.2352	399906.1	-25.4743
					10000	0.40	40.0	5026.5	147.0705	739257.0	-1.3698
					10000	0.40	60.0	11309.7	139.15781	573837.1	0.1535
					10000	0.40	80.0	20106.2	103.82462	807518.1	0.0350
					10000	0.40	100.0	31415.9	85.01602	670855.0	0.0119

PROGRAM PACKEDBED3

This program uses Eq. (13) to calculate outlet concentration and Eq. (21) to calculate pressure drop for a specified bed. The program listing is shown in Table D-6. PACKEDBED3 has teletype I/O. Upon compiling and executing the controller (see Table D-7), the message "ENTER DATA" is printed. Then, on the next line a "?" is printed. Any piece of data can be entered by typing one of the following three-letter codes, followed by the number in F20.10 format:

TMP temperature (°C)
 PRS pressure (atm)
 EPS bed-void fraction
 BDS number of beds splitting total flow
 DP getter particle diameter (μm)
 L/D length-to-diameter (ratio of bed)
 RAD bed radius (cm)
 RUN execute program with current set of data
 END terminate program.

After entering a code and value, "?" will be repeated, asking for more data. Codes and values may be entered in any order; if more than one value for one code is entered, the last is used. If a code other than one of those above is entered, a message to that effect is printed and the entry is ignored.

When "RUN" is entered, a check is made to see that all values have been defined; if one has not, the three-character code is printed followed by "?". A value for this code must be entered before execution can begin.

When the "RUN" command is given and all variables have been defined, the bed pressure drop is calculated and printed, the outlet concentration in mole/cm³ and ppm is calculated and printed, and the approach to equilibrium as defined by

$$\text{Approach} = \left(\frac{c_f - c_s}{c_o - c_s} \right) \quad (\text{D-2})$$

is printed. Then "ENTER DATA" is printed, followed by "?". Any or all parameter values can be changed; if a parameter is not redefined, the old value is retained.

If the bed pressure drop is larger than the inlet pressure, a message to this effect is printed and new data are requested by a "?". If the algorithm does not converge, the message "NO CONVERGENCE" is printed and new data are requested by "ENTER DATA" and "?".

Entering "END" terminates the program at any time.

Table D-6. PACKBED3 listing.

```

PROGRAM PACKEDBEO3(TAPE59)
REAL M,LDRATIO,L,MU,J,D,KX
DIMENSION VALUE(9),NAME(9)
EQUIVALENCE (T,VALUE(1)),(P,VALUE(2)),(EPS,VALUE(3)),&
(M,VALUE(4)),(DP,VALUE(5)),(LDRATIO,VALUE(6)),(RAD,VALUE(7))
DATA NAME / "TMP","PRS","EPS","BDS","DP","L/D","RAD",&
"RUN","END"/
T=P=EPS=M=DP=LDRATIO=RAD=VALUER=0.0
NAME=""
CALL CHANGE(4R+ABC)
WRITE(59,"(//"" ENTER DATA""/")")
DO 1 I=1,7
READ(59,"(A3,F20.10)")NAME,VALUER
IF(NAME.NE.NAME(I))GO TO 5
IF(I.EQ.1)VALUER=VALUER+273.
IF(I.EQ.5)VALUER=VALUER+1.0E-4
VALUE(I)=VALUER
GO TO 1
CONTINUE
IF(NAME.EQ.NAME(8))GO TO 2
IF(NAME.EQ.NAME(9))CALL EXIT
WRITE(59,"(" INCDRECT ENTRY - "",A3)" )NAME
GO TO 1
DO 3 I=1,7
IF(VALUE(I).NE.0.0)GO TO 3
WRITE(59,"(" "" ,A3,"" ?"" )" )NAME(I)
GO TO 1
CONTINUE
COMPUTE DELP,DELC
CO=4.63E-6*P/T
CU=(10.*(10.72-10840./T))/(62363.*T)
MS=17.78E-5*(4.58*T/151.-1.67)*0.625)*1.0E-2/0.02763
AA=E.O.(1-C-EPS)/DP
RH=E.P*-454./(1.314*T*((2.54*12.).**3))
C1=RH*1/40.
F1=1.0E7/(M*P)
DAB1=1.524E-5*(T**1.823)/P
I=0
J=0
A=3.141592654*RAD=RAD
RH01B=RH01
C1B=C1
F1B=F1
V1B=F1B/A
DAB1B=DAB1
GO=17845.7/(M*A)
RE=GO/(AA*MU)
IF(RE.LE.50.0)GO TO 101
JD=0.61*(RE**(-0.41))
GO TO 102
JD=0.91*(RE**(-0.51))
CONTINUE
TEMP2=((150.*(1.0-EPS)/(DP*GO/MU)+1.75)*(1.0-EPS)*GO*GO/&
(DP*EPS**3))*(.1.4504E-5/14.7)
KX=JD*V1B*C1B*((DAB1B*RH01B/MU)**(2.0/3.0))
I=1
L=LDRATIO*2.0/RAD
TEMP3=(-AA*KX*62363.*T*(L-.6/(A*M*EPS*0.0115)))/(F1*760.*P)
CONFZ=CS+(CO-CS)*EXP(TEMP3)

```

Table D-6. (Continued)

```

61 DELP=TEMP2*L/RHO1B
62 IF(DELP,LE,P)GO TO 104
63 WRITE(59,*)
64 "(/" PRESSURE DROP IS LARGER THAN INPUT PRESSURE")")
65 GO TO 1
104 RHO2B=RHO1*(2.0*P-DELP)/(2.0*P)
66 F2B=F1*(2.0*P-DELP)/(2.0*(P-DELP))
67 V2B=F2B/A
68 DAB2B=DAB1*(2.0*P-DELP)/(2.0*(P-DELP))
69 IF(1.GT.500)GO TO 150
70 IF(ABS((V1B-V2B)/V1B).GT.1.0E-2)GO TO 115
71 IF(ABS((RHO1B-RHO2B)/RHO1B).GT.1.0E-2)GO TO 115
72 IF(ABS((DAB1B-DAB2B)/DAB1B).LE.1.0E-2)GO TO 120
73 V1B=V2B
115 F1B=F2B
74 DAB1B=DAB2B
75 RHO1B=RHO2B
76 C1B=RHO1B/40.
77 GO TO 105
78
120 APPR=(COFZ-CS)/(CO-CS)
81 PPM=COFZ*3.8/CO
82 WRITE(59,")(/" BED PRESSURE DROP, ATM"" F10.4)")DELP
83 WRITE(59,")(" C OUT, MOLES/CC "" E15.4)"COFZ
84 WRITE(59,")(" C OUT, PPM"" E15.4)"PPM
85 WRITE(59,")(" APPROACH "" E15.4)"APPR
86 GO TO 10
150 WRITE(59,")(" NO CONVERGENCE")")
87 GO TO 10
88
89 END

```

Table D-7. PACKBED3 compilation and execution.

Compile and create controllee

```
CHAT PACKEDBED3 P300 P3BIN P3LIS1 Y02 M M / 1 1.4
LOADING
CODE BLOC          P3G0 WRITTEN
FILE SIZE=        0013347
FLD LGTH=         0013117  0011112
```

Execute controllee

P3G0 / 1 1

ENTER DATA

?
TMP 25.0

?
PRS 1.0

?
EPS 0.4

?
BDS 1.0

?
DP 100.0

?
L/D 0.1

?
RAD 100.0

?
RUN
INCORRECT ENTRY - RUN

?
RUN

PRESSURE DROP IS LARGER THAN INPUT PRESSURE
?

RAD 200.0
?

RUN

PRESSURE DROP IS LARGER THAN INPUT PRESSURE
?

L/D .001
?

RUN

```
BED PRESSURE DROP, ATM      0.0755
C OUT, MOLES/CC             1.188E-33
C OUT,PPM                   2.9069E-23
APPROACH                     0.
```

ENTER DATA

?
L/D .01

?
RUN

PRESSURE DROP IS LARGER THAN INPUT PRESSURE
?

FND

ALL DONE

Appendix E: Computer Program for Fluidized-Bed Modeling

PROGRAM FLUIDBED1

This program predicts fluidized-bed reactor performance for parameters specified in teletype input; parameters may be varied after each case is calculated. The perforated-plate specification is the number of holes in the plate.

FLUIDBED1 has teletype I/O. A listing of the program is given in Table E-1. Upon compiling and executing, the controller (see Table E-2) the message "ENTER DATA" is printed. Then, on the next line, a "?" is printed. Any parameter may be entered by typing one of the three-letter codes below followed by the parameter in F20.10 format:

TMP	temperature (°C)
PRS	inlet pressure (atm)
PRF	number of holes in perforated plate
BDS	number of beds dividing the total flow
RAD	radius of bed (cm)
DPS	getter particle diameter (μm)
EMF	bed-void fraction at minimum fluidization
GWT	weight of getter in bed (g)
RUN	execute program with current set of parameters
END	terminate program.

After entering a code and value, "?" will be repeated, asking for more data. Codes and values may be entered in any order. If more than one value for a code is entered, the last is used. If an unknown code is entered, a message to that effect is printed, and the entry is ignored.

When "RUN" is entered, a check is made to see that all variables have been defined. If one has not, the three-character code is printed followed by a "?." A value for this parameter must be entered before execution will be successful.

When "RUN" is entered and all variables have been defined, the question "VARY DELTA?" is printed. If "YES" is entered, the bed calculations will be made for $\delta = 0.1(D_p/2)$, $(D_p/2)$, and $\delta = 10 (D_p/2)$. If anything else is entered, calculations will be made only for $\delta = (D_p/2)$.

After calculating bed performance, four or five lines of output are printed. If the parameters allow use of the model, the first line will be "N = I," where I is an integer giving the total number of compartments in the bed. If the model cannot be used, this line will not be printed.

The next four lines of output are always given. The first gives the inlet and outlet concentrations in parts per million. The second line gives the gas velocity, the minimum allowable velocity (u_{mf}), and the maximum allowable velocity (u_p), all in cm/s. The third line gives the length of the bed during normal operation (L), and the length of the bed at minimum fluidization velocity (LMF), both in cm. The fourth line gives the bed pressure drop in atmospheres and the theoretical power needed to pump it with a 100% efficient compressor.

After printing the four or five lines of output (three times, if δ is varied; first for the smallest δ , last for the largest δ), "ENTER DATA" is printed. Any code and value can be entered, and the program rerun.

Entering "END" terminates the program.

For some cases, the outlet concentration will be equal to the inlet concentration. This reflects an approximation in the model, and arises from two factors. First, for too many perforations in the plate, the lower compartments are filled entirely with bubbles (i.e., no emulsion phase is present, so no reaction occurs). Second, at the top of the bed where the solids are very dispersed, essentially no reaction occurs. For some sets of parameters, the intermediate compartments where reaction would occur are not present. To correct this condition, either decrease the number of holes or increase the amount of getter in the bed.

If the model is not applicable, the outlet concentration, bed lengths, pressure drop, and pumping power will all equal either -1, -2, -3, or -4. If they equal -1, the gas velocity is less than the minimum fluidization velocity; -2 indicates that the gas velocity is larger than the maximum velocity allowable. Values of -3 indicate that the bubbles are too small or the getter particles too big for the model. Values of -4 means that the product $(DP + u/u_{mf})$ is too large for the model to handle.

Table E-1. FLUIDBED1 listing.

```

1 PROGRAM FLUIDBED1(TAPE59)
2 REAL M,L,LMF
3 DIMENSION VALUE(8),INAME(10)
4 VALUE(4)=T,VALUE(1),(P,VALUE(2)),(M,VALUE(3)),(HOLES,&
5 VALUE(4)),RAD,VALUE(5),(DP,VALUE(6)),(EMF,VALUE(7)),&
6 (CEWT,VALUE(8))
7 DATA INAME/'TMP','PRS','BDS','PRF','RAD','OPS','EMF',&
8 'GWT','RUN','END'/
9 COMMON /FLUID1/ L,LMF,UMF,UT,U,CIN,COUT,CPPM1,CPPM5,DELP,&
10 POWER,DELTA
11 CALL CHANGE(4R+XYZ)
12 T=EMF=M=DP=CEWT=HOLES=RAD=VALUER=0.0
13 NAME=""
14 C ENTER DATA
15 1 WRITE(59,/'( " ENTER DATA" )')
16 2 WRITE(59,/'( " ?" )')
17 READ (59,/'(A3,F20.10)')NAME,VALUER
18 DO 3 I=1,8
19 IF(NAME.NE.INAME(I))GO TO 3
20 IF(I.EQ.1)VALUER=VALUER+273.C
21 IF(I.EQ.6)VALUER=VALUER+1.0E-4
22 VALUE(I)=VALUER
23 GO TO 2
24 3 CONTINUE
25 IF(NAME.EQ.INAME(9))GO TO 4
26 IF(NAME.EQ.INAME(10))CALL EXIT
27 WRITE(59,/'( " INCORRECT ENTRY - " ,A3)')NAME
28 GO TO 2
29 4 DO 5 I=1,8
30 IF(VALUE(I).NE.0.0)GO TO 5
31 WRITE(59,/'( " " ,A3, " ?" )')INAME(I)
32 GO TO 2
33 5 CONTINUE
34 WRITE(59,/'( " VARY DELTA?" )')
35 READ(59,/'(A3)')NAME
36 DELT=DP/2.0
37 DO 10 I=1,3
38 IF(NAME.NE."YES".AND.I.NE.2)GO TO 10
39 DELTA=DELT*(10.0*(I-2))
40 CALL FLUID(T,P,M,HOLES,RAD,DP,EMF,CEWT)
41 C OUTPUT DATA
42 WRITE (59,1000)CPPM1,CPPM5
43 1000 FORMAT(/'INLET CONC.=',E11.4 PPM OUTLET CONC.=',E11.4," PPM")
44 WRITE(59,1001)U,UMF,UT
45 1001 FORMAT('VELOCITIES: U= ",E11.4," UMF= ",E11.4," UT= ",E11.4)
46 WRITE (59,1002)LMF
47 1002 FORMAT('BED LENGTHS: L= ",E11.4," LMF= ",E11.4)
48 WRITE (59,1003)DELP,POWER
49 1003 FORMAT('BED PRES. DROP OF ",F6.3," ATM REQUIRES ",E11.4,&
50 " KW POWER")
51 10 CONTINUE
52 GO TO 1
53 END

1 SUBROUTINE FLUID(T,P,M,HOLES,RAD,DP,EMF,CEWT)
2 REAL M,LMF,MU,K,L
3 COMMON /FLUID1/L,LMF,UMF,UT,U,CIN,COUT,CPPM1,CPPM5,DELP,&
4 POWER,DELTA
5 P1=3.141592654
6 RHOP=6.7
7 RHOGIN=40.0*P/(82.057*T)
8 CPMM1=3.8
9 CIN=(RHOGIN/40.0)*CPPM1*1.0E-6
10 VMF=CEWT/(RHOP*(1.0-EMF))
11 A=RAD=RAD*PI
12 LMF=VMF/A
13 MU=17.78E-5*((4.58*T/151.-1.67)*0.625)+1.0E-2/0.02763
14 UMF=(SQRT(33.7*33.7+0.0408*DP*DP*DP*DP*RHOGIN*(RHOGIN)*&
15 980./(MU*U))-33.7)*MU/(DP*RHOGIN)
16 UT=980.*DP*DP*(RHOP-RHOGIN)/(18.0*MU)
17 REP=DP*RHOGIN=UT/MU
18 IF(REP.LE.0.4)GO TO 10
19 UT=(4.0/225.0)*((RHOP-RHOGIN)*(RHOP-RHOGIN)*980.*980./&
20 (RHOGIN*MU))*((3.0)*DP
21 REP=DP*RHOGIN=UT/MU
22 IF(REP.LE.500.10)*5 10
23 UT=SQRT(3.1*980.*(RHOP-RHOGIN)*DP/RHOGIN)
24 REP=DP*RHOGIN=UT/MU
25 IF(REP.LE.2.0E+05)GO TO 10

```

Table E-1. (Continued)

```

26 WRITE(59, "(" " UT?" " ", 2E15.4) ) REP, UT
27 CONTINUE
28 F=1.0E7/(M=P)
29 U=F/A
30 DAB=1.524E-5*(T**1.823)/P
31 G=(U-UMF)/H0LES
32 IF(U.LT.UMF) GO TO 500
33 DO=((6.0*G/P)**0.4)/(980.0**0.2)
34 DB=DO
35 DBBAR=1.4*RHO*DP*(U/UMF)*(LMF/2.0)+DO
36 L=(U-UMF)/(0.711*SQR(DBBAR*980.0))*LMF+LMF
37 CONST=1.4*RHO*DP*U/UMF
38 H=0.0
39 N=0
40 EPS=1.0-LMF*(1.0-EMF)/L
41 CBNM1=CIN
42 IF(U.GE.UT) GO TO 800
43 IF(CONST.GE.2.0) GO TO 600
100 N=N+1
44 DELHN=2.0*DO*((2.0+CONST)**(N-1))/(2.0-CONST)**N
45 H=H+DELHN
46 IF(H.LT.LMF) GO TO 101
47 EPS=(1.0-LMF*(1.0-EMF)/L)+LMF*(1.0-EMF)*(H-LMF)/(2.0*L*(L-LMF))
48 IF(EPS.GT.1.0) EPS=1.0
101 AA=6.0*(1.0-EPS)/DP
49 K=DAB/AA/DELTA
50 UB=0.711*SQR(DELHN*980.0)
51 IF(UB.LE.UMF/EMF) GO TO 700
52 CAPN=6.0*A*(L-LMF)/(PI*L*DELHN*DELHN)
53 CONST2=CAPN*PI*DELHN*DELHN/DELHN/(6.0*(UB-UMF/EMF))
54 VBN=CONST2*3.0*UMF/EMF
55 VBN=CONST2*(UB+2.0*UMF/EMF)
56 VEN=A*DELHN-VBN
57 IF(VEN.GE.0.0) GO TO 102
58 VEN=0.0
61 VBN=A*DELHN
102 CONTINUE
62 DB=CONST*H+DO
63 FONP=((1.0/DB)*(UB-UMF/EMF)/(UB+2.0*UMF/EMF))
64 CBN=((4*U+CIN)/(FONP*VBN*(1.0-FONP*VBN/(K*VEN+FONP*VBN))))*
65 K*VEN*A*U
66 CBN=CIN/(FONP*VBN*(K*VEN+FONP*VBN))
67 IF(H.GE.(LMF+2.0*(L-LMF))) GO TO 105
68 CBNM1=CBN
69 GO TO 100
71 COUT=CBN
105 CPPMO=CBN*1.0E+06*(RHOGIN/40.0)
72 WRITE(59, "(" " N = " ", 110) " ) N
73 GAMMA=.6667
74 DELP=(1.0-EMF)*(RHO*P-RHOGIN)*980.0*LMF*9.8692E-7
75 P2=P-DELP
76 IF(P2.GE.0.0) GO TO 106
77 POWER=-0.0
78 GO TO 110
106 POWER=-GAMMA/(GAMMA-1.0)*10.0E+6*((P2/P)**((GAMMA-1.0)/GAMMA))&
81 -1.0)*1.0E-3*74.74*0.0013558
82 110 CONTINUE
83 RETURN
84 500 CPPMO=L=LMF=DELP=POWER=-1.0
85 RETURN
86 600 CPPMO=L=LMF=DELP=POWER=-4.0
87 RETURN
88 700 CPPMO=L=LMF=DELP=POWER=-3.0
89 RETURN
90 800 CPPMO=L=LMF=DELP=POWER=-2.0
91 RETURN
92 END

```

Table E-2. FLUIDBED1 compilation and execution.

Compile and create controllee

```
CHAT FLUIDBED1 FIGO FIBIN FILIST Y02 M M / 1 1.4
LOADING
CODE BLOC          FIGO WRITTEN
FILE SIZE=        0014306
FLD LGTH=         0014056   0012051
```

ALL DONE

Execute controllee

FIGO / 1 1

ENTER DATA

?

TMP 25.0

?

PRS 1.0

?

PRF 10000.

?

RAD 200.

?

DPS 100.0

?

EMF .5

?

GWT 100000.

?

RUN

BDS ?

?

BDA C.

INCORRECT ENTRY - BDA

?

BDS 2.

?

RUN

VARY DELTA?

NO

```
INLET CONC.= 3.0000E+00 PPM      OUTLET CONC.= -4.0000E+00 PPM
VELOCITIES: U= 3.9789E+01 UMF= 1.7489E+00 U1= 1.2783E+02
BED LENGTHS: L= -4.0000E+00 LMF= -4.0000E+00
BED PRES. DROP OF -4.000 ATM REQUIRES -4.0000E+00 KW POWER
```

ENTER DATA

?

RAD 300.0

?

RUN

VARY DELTA?

NO

N = 4

```
INLET CONC.= 3.0000E+00 PPM      OUTLET CONC.= 3.0000E+00 PPM
VELOCITIES: U= 1.7684E+01 UMF= 1.7689E+00 U1= 1.2783E+02
BED LENGTHS: L= 3.8247E-01 LMF= 1.0558E-01
BED PRES. DROP OF 0.000 ATM REQUIRES 3.4658E-01 KW POWER
```

ENTER DATA

?

GWT 250000.

?

RUN

Table E-2. (Continued)

```

VARY DELTA?
NO
N = 4

INLET CONC.= 3.8000E+00 PPM      OUTLET CONC.= 3.8000E+00 PPM
VELOCITIES: U= 1.7684E+01 UMF= 1.7689E+00 U1= 1.2783E+02
BED LENGTHS: L= 7.5355E-01 LMF= 2.4394E-01
BED PRES. DROP OF 0.001 ATM REQUIRES 8.6658E-01 KW POWER

ENTER DATA
?
PRF 5000.
?
RUN
VARY DELTA?
NO
N = 4

INLET CONC.= 3.8000E+00 PPM      OUTLET CONC.= 3.8000E+00 PPM
VELOCITIES: U= 1.7684E+01 UMF= 1.7689E+00 U1= 1.2783E+02
BED LENGTHS: L= 7.4098E-01 LMF= 2.6394E-01
BED PRES. DROP OF 0.001 ATM REQUIRES 8.6658E-01 KW POWER

ENTER DATA
?
GWT 100000.
?
RUN
VARY DELTA?
NO
N = 5

INLET CONC.= 3.8000E+00 PPM      OUTLET CONC.= 1.0220E+03 PPM
VELOCITIES: U= 1.7684E+01 UMF= 1.7689E+00 U1= 1.2783E+02
BED LENGTHS: L= 2.0949E+00 LMF= 1.0558E+00
BED PRES. DROP OF 0.003 ATM REQUIRES 3.4690E+00 KW POWER

ENTER DATA
?
PRF 100000.
?
RUN
VARY DELTA?
NO

INLET CONC.= 3.8000E+00 PPM      OUTLET CONC.= -3.0000E+00 PPM
VELOCITIES: U= 1.7684E+01 UMF= 1.7689E+00 U1= 1.2783E+02
BED LENGTHS: L= -3.0000E+00 LMF= -3.0000E+00
BED PRES. DROP OF -3.000 ATM REQUIRES -3.0000E+00 KW POWER

ENTER DATA
?
PRF 5000.
?
RAD 100.
?
RUN
VARY DELTA?
NO

INLET CONC.= 3.8000E+00 PPM      OUTLET CONC.= -2.0000E+00 PPM
VELOCITIES: U= 1.5915E+02 UMF= 1.7689E+00 U1= 1.2783E+02
BED LENGTHS: L= -2.0000E+00 LMF= -2.0000E+00
BED PRES. DROP OF -2.000 ATM REQUIRES -2.0000E+00 KW POWER

ENTER DATA
?

```

Table E-2. (Continued)

```

-
RAD 300.
?
RUN
VARY DELTA?
YES
N = 5

INLET CONC.= 3.8000E+00 PPM      OUTLET CONC.= 1.0799E-05 PPM
VELOCITIES: U= 1.7684E+01 UMF= 1.7689E+00 UT= 1.2783E+02
BED LENGTHS: L= 2.0949E+00 LMF= 1.0558E+00
BED PRES. DROP OF 0.003 ATM REQUIRES 3.4690E+00 KW POWER
N = 5

INLET CONC.= 3.8000E+00 PPM      OUTLET CONC.= 1.0228E-03 PPM
VELOCITIES: U= 1.7684E+01 UMF= 1.7689E+00 UT= 1.2783E+02
BED LENGTHS: L= 2.0949E+00 LMF= 1.0558E+00
BED PRES. DROP OF 0.003 ATM REQUIRES 3.4690E+00 KW POWER
N = 5

INLET CONC.= 3.8000E+00 PPM      OUTLET CONC.= 6.5718E-02 PPM
VELOCITIES: U= 1.7684E+01 UMF= 1.7689E+00 UT= 1.2783E+02
BED LENGTHS: L= 2.0949E+00 LMF= 1.0558E+00
BED PRES. DROP OF 0.003 ATM REQUIRES 3.4690E+00 KW POWER

ENTER DATA
?
END

ALL DONE

```

PROGRAM FLUIDBED2

This program uses the same set of parameters and same calculational methods as FLUIDBED1, but carries out the calculations for specified values of parameters. For the listing given here (Table E-3), the parameters are varied as follows:

$T = 523 \text{ K}$

$DP = 100 \text{ }\mu\text{m}$

$P = 5, 10 \text{ atm}$

Number of beds = 2, 5, 10

Number of perforations in plate = $10^2, 10^3, 10^4$

$EMF = 0.4, 0.5, 0.6$

$RAD = 0.50, 1.00, 1.50, 2.00 \text{ m}$

$GWT = 1.0, 5.0, 10.0, 50.0 \text{ kg}$

$\delta = 0.1, 1, 10 \text{ times } DP/2.$

Program output is directed to a high-speed printer.

Following the program listing in Table E-3 is an example of the program being compiled and executed (Table E-4). Before execution starts, the query "RUN" is printed. To execute, enter "YES"; anything else terminates the program. When the program is complete, it prints "DONE."

One page of output is shown in Table E-5; 65 pages are generated. At the top of each page are printed parameters which have constant value for that page. Then, for all values of radius, getter weight, and film thickness, seven columns of data are given: outlet concentration (ppm), gas velocity in reactor $u(\text{cm/s})$, minimum fluidization velocity $u_{mf}(\text{cm/s})$, length of bed $L(\text{cm})$, length of bed at minimum fluidization $L_{MF}(\text{cm})$, pressure drop in bed $DEL P(\text{atm})$, and theoretical pumping power $POWER(\text{kW})$. At the bottom of the page, the maximum bed velocity (or terminal velocity of particles) is given, followed by the meanings of the output values -1, -2, -3, and -4.

Table E-3. FLUIDBED2 listing.

```

1      PROGRAM FLUIDBED2(HSP)
2      PROGRAM FLUIDOUT1(FOUT,UT,TAPE3=FOUTPUT)
3      REAL M,L,LMF
4      COMMON /FLUID1/ L,LMF,UMF,UT,U,CIN,COUT,CPPMI,CPPMO,
5      1 DELP,POWER,DELTA
6      DIMENSION CEW(4)
7      DATA CEW/1000.,5000.,10000.,50000./
8      CALL CHANGE(4R+MNO)
9      INAME="
10     T=523
11     DP=0.01
12     DP1=DP*1.0E+4
13     WRITE(59,("( " RUN?""))
14     READ(59,("(A3)"))INAME
15     IF(INAME.NE."YES")CALL EXIT
16     DO 1 IP=5,10,5
17     DO 1 IM=1,3
18     M=3.0*IM-1.0
19     IF(IM.EQ.3)M=10.0
20     DO 1 IH=1,3
21     HOLES=10.0*=(IH+1)
22     DO 1 IE=4,6
23     EMF=0.1*IE
24     WRITE(3,100)T,P
25     100 FORMAT(41," T= ",F5.1," DEG. K",15X,"P= ",F4.1," ATM")
26     WRITE(3,101)M,HOLES
27     101 FORMAT(4," NUMBER OF BEDS = ",F4.0,20X,&
28     2 "NUMBER OF HOLES IN DISTRIBUTOR PLATE = ",F7.0)
29     WRITE(3,102)DP1,EMF
30     102 FORMAT(4," BETTER PARTICLE DIAMETER = ",F7.1," MICRONS",10X,&
31     3 "BED VOID FRACTION AT MIN. FLUID. COND. = ",F7.3)
32     WRITE(3,103)
33     103 FORMAT(73X,"RAD",5X,"CEWT",3X,"DELTA",4X,"C OUT PPM",8X,&
34     4 "U",11X,"UMF",11X,"L",11X,"LMF",10X,"DELP",9X,"POWER"/)
35     DO 2 IR=50,200,50
36     RAD=IR
37     DO 2 IC=1,4
38     CEWT=CEW(IC)
39     DO 2 ID=1,3
40     DELTA=(DP/2.0)*10.0*=(ID-2)
41     CALL FLUID(T,P,M,HOLES,RAD,DP,EMF,CEWT)
42     WRITE(3,104)RAD,CEWT,DELTA,CPPMO,U,UMF,L,LMF,DELP,POWER
43     104 FORMAT(15,F9.1,F8.4,7E13.4)
44     WRITE(3,105)UT
45     105 FORMAT(7," TERMINAL VELOCITY = ",E13.4)
46     WRITE(3,106)
47     106 FORMAT(7," -1.0: U .LT. UMF",20X,"-2.0: U .GT. UT"/&
48     8 " -3.0: UB .LE. UMF/EMF",15X,"-4.0: CONST .GT. 2, DELH .LT. 0")
49     1 CONTINUE
50     WRITE(59,("( " DONE""))
51     CALL EXIT
52     END
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Table E-3. (Continued)

```

25 F=1.0E7/(M*P)
26 U=F/A
27 DAB=1.524E-5*(T==1.823)/P
28 G=(U-UMF)/HOLDS
29 IF(U.LT.UMF)GO TO 500
30 DO=((6.0*G/P1)**0.4)/(980.0**0.2)
31 DB=DO
32 DBBAR=1.4*RHOP*DP*(U/UMF)*(LMF/2.0)+DO
33 L=(U-UMF)/(0.711*SQRT(DBBAR*980.0))*LMF+LMF
34 CONST=1.4*RHOP*DP*U/UMF
35 H=0.0
36 N=0
37 EPS=1.0-LMF*(1.0-EMF)/L
38 CBNM1=CIN
39 IF(U.GE.UT)GO TO 800
40 IF(CONST.GE.2.0)GO TO 600
41 N=N+1
42 100 NELHN=2.0*DO*((2.0+CONST)**(N-1))/((2.0-CONST)**N)
43 H=H+DELHN
44 IF(H.LT.LMF)GO TO 101
45 EPS=1.-(LMF*(1.0-EMF)/L)+LMF*(1.0-EMF)*(H-LMF)/(2.0*L*(L-LMF))
46 IF(EPS.GT.1.0)EPS=1.0
47 101 AA=6.0*(1.0-EPS)/DP
48 K=DAB*AA/DELTA
49 UB=0.711*SQRT(DELHN*980.0)
50 IF(UB.LE.UMF/EMF)GO TO 700
51 CAPN=6.0*A*(L-LMF)/(P1*L*DELHN*DELHN)
52 CONST2=CAPN*P1*DELHN*DELHN/DELHN/(6.0*(UB-UMF/EMF))
53 VCN=CONST2*3.0*UMF/EMF
54 VBN=CONST2*(UB+2.0*UMF/EMF)
55 VEN=A*DELHN-VBN
56 IF(VEN.GE.0.0)GO TO 102
57 VEN=0.0
58 VBN=A*DELHN
59 102 CONTINUE
60 UB=CONST*H+DO
61 FONP=(11.0/DB)*(UB-UMF/EMF)/(UB+2.0*UMF/EMF)
62 CBN=(A*U*CBNM1)/(FONP*VBN*(1.0-FCNP*VDN/(K*VEN+FONP*VBN)))+G
63 K=VEN+A*U
64 CEN=FCIF*VBN*CBN/(K*VEN+FONP*VBN)
65 IF(H.GE.(LMF+2.0*(L-LMF)))GO TO 105
66 CBNM1=CBN
67 GO TO 100
68 105 COUT=CBN
69 CPPMO=CBN*1.0E+06/(RHODIN/40.0)
70 GAMMA=1.6667
71 DELP=(1.0-EMF)*(RHOP-RHODIN)*980.0*LMF*9.8692E-7
72 P2=P-DELP
73 IF(P2.GE.0.0)GO TO 106
74 POWER=-0.0
75 GO TO 110
76 106 POWER=-GAMMA/(GAMMA-1.0)*10.0E+6*((P2/P)**((GAMMA-1.0)/GAMMA))-1.0*1.0E-3*74.74*0.0013558
77 110 CONTINUE
78 RETURN
79 500 CPPMO=L*LMF=DELP=POWER=-1.0
80 RETURN
81 600 CPPMO=L*LMF=DELP=POWER=-4.0
82 RETURN
83 700 CPPMO=L*LMF=DELP=POWER=-3.0
84 RETURN
85 800 CPPMO=L*LMF=DELP=POWER=-2.0
86 RETURN
87 END
88
89

```

Table E-4. FLUIDBED2 compilation and execution.

Compile, create, and execute controllee

```
CHAT FLUIDBED2 F2605 F2BIN F2LIST Y02 M M / 1 1.4
LOADING
CODE BLOC      F260 WRITTEN
FILE SIZE=     0014315
FLD LGTH=      0014065    0012060
EXECUTION
RUN?
YES
DONE

ALL DONE
```

Table E-5. Example of FLUIDBED2 output.

1 T= 523.0 DEG. K			P= 5.0 ATM			NUMBER OF HOLES IN DISTRIBUTOR PLATE = 100.			BED VOID FRACTION AT MIN. FLUID COND. = 0.400		
NUMBER OF BEDS = 2			GETTER PARTICLE DIAMETER = 100.0 MICRONS								
RAD	CEWT	DELTA	C OUT PPM	U	UMF	L	LMF	DELP	POWER		
50.0	1000.0	0.0005	3.8000E+00	1.2732E+02	1.1732E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00
50.0	1000.0	0.0050	3.8000E+00	1.2732E+02	1.1732E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00
50.0	1000.0	0.0500	3.8000E+00	1.2732E+02	1.1732E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00
50.0	5000.0	0.0005	3.8000E+00	1.2732E+02	1.1732E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00
50.0	5000.0	0.0050	3.8000E+00	1.2732E+02	1.1732E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00
50.0	5000.0	0.0500	3.8000E+00	1.2732E+02	1.1732E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00
50.0	10000.0	0.0005	3.8000E+00	1.2732E+02	1.1732E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00
50.0	10000.0	0.0050	3.8000E+00	1.2732E+02	1.1732E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00
50.0	10000.0	0.0500	3.8000E+00	1.2732E+02	1.1732E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00
50.0	50000.0	0.0005	3.8000E+00	1.2732E+02	1.1732E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00
50.0	50000.0	0.0050	3.8000E+00	1.2732E+02	1.1732E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00
50.0	50000.0	0.0500	3.8000E+00	1.2732E+02	1.1732E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00	-2.0000E+00
100.0	1000.0	0.0005	3.8000E+00	3.1831E+01	1.1732E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00
100.0	1000.0	0.0050	3.8000E+00	3.1831E+01	1.1732E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00
100.0	1000.0	0.0500	3.8000E+00	3.1831E+01	1.1732E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00
100.0	5000.0	0.0005	3.8000E+00	3.1831E+01	1.1732E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00
100.0	5000.0	0.0050	3.8000E+00	3.1831E+01	1.1732E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00
100.0	5000.0	0.0500	3.8000E+00	3.1831E+01	1.1732E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00
100.0	10000.0	0.0005	3.8000E+00	3.1831E+01	1.1732E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00
100.0	10000.0	0.0050	3.8000E+00	3.1831E+01	1.1732E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00
100.0	10000.0	0.0500	3.8000E+00	3.1831E+01	1.1732E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00
100.0	50000.0	0.0005	3.8000E+00	3.1831E+01	1.1732E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00
100.0	50000.0	0.0050	3.8000E+00	3.1831E+01	1.1732E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00
100.0	50000.0	0.0500	3.8000E+00	3.1831E+01	1.1732E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00	-4.0000E+00
150.0	1000.0	0.0005	3.8000E+00	1.4147E+01	1.1732E+00	8.8817E-03	3.5192E-03	1.3673E-05	2.7711E-03	1.3673E-05	2.7711E-03
150.0	1000.0	0.0050	3.8000E+00	1.4147E+01	1.1732E+00	8.8817E-03	3.5192E-03	1.3673E-05	2.7711E-03	1.3673E-05	2.7711E-03
150.0	1000.0	0.0500	3.8000E+00	1.4147E+01	1.1732E+00	8.8817E-03	3.5192E-03	1.3673E-05	2.7711E-03	1.3673E-05	2.7711E-03
150.0	5000.0	0.0005	3.8000E+00	1.4147E+01	1.1732E+00	4.3707E-02	1.7596E-02	6.8367E-05	1.3856E-02	6.8367E-05	1.3856E-02
150.0	5000.0	0.0050	3.8000E+00	1.4147E+01	1.1732E+00	4.3707E-02	1.7596E-02	6.8367E-05	1.3856E-02	6.8367E-05	1.3856E-02
150.0	5000.0	0.0500	3.8000E+00	1.4147E+01	1.1732E+00	4.3707E-02	1.7596E-02	6.8367E-05	1.3856E-02	6.8367E-05	1.3856E-02
150.0	10000.0	0.0005	3.8000E+00	1.4147E+01	1.1732E+00	8.5808E-02	3.5192E-02	1.3673E-04	2.7711E-02	1.3673E-04	2.7711E-02
150.0	10000.0	0.0050	3.8000E+00	1.4147E+01	1.1732E+00	8.5808E-02	3.5192E-02	1.3673E-04	2.7711E-02	1.3673E-04	2.7711E-02
150.0	10000.0	0.0500	3.8000E+00	1.4147E+01	1.1732E+00	8.5808E-02	3.5192E-02	1.3673E-04	2.7711E-02	1.3673E-04	2.7711E-02
150.0	50000.0	0.0005	3.8000E+00	1.4147E+01	1.1732E+00	3.8366E-01	1.7596E-01	6.8367E-04	1.3856E-01	6.8367E-04	1.3856E-01
150.0	50000.0	0.0050	3.8000E+00	1.4147E+01	1.1732E+00	3.8366E-01	1.7596E-01	6.8367E-04	1.3856E-01	6.8367E-04	1.3856E-01
150.0	50000.0	0.0500	3.8000E+00	1.4147E+01	1.1732E+00	3.8366E-01	1.7596E-01	6.8367E-04	1.3856E-01	6.8367E-04	1.3856E-01
200.0	1000.0	0.0005	3.8000E+00	7.9577E+00	1.1732E+00	3.7825E-03	1.9795E-03	7.6912E-06	1.5587E-03	7.6912E-06	1.5587E-03
200.0	1000.0	0.0050	3.8000E+00	7.9577E+00	1.1732E+00	3.7825E-03	1.9795E-03	7.6912E-06	1.5587E-03	7.6912E-06	1.5587E-03
200.0	1000.0	0.0500	3.8000E+00	7.9577E+00	1.1732E+00	3.7825E-03	1.9795E-03	7.6912E-06	1.5587E-03	7.6912E-06	1.5587E-03
200.0	5000.0	0.0005	3.8000E+00	7.9577E+00	1.1732E+00	1.8813E-02	9.8977E-03	3.8456E-05	7.7937E-03	3.8456E-05	7.7937E-03
200.0	5000.0	0.0050	3.8000E+00	7.9577E+00	1.1732E+00	1.8813E-02	9.8977E-03	3.8456E-05	7.7937E-03	3.8456E-05	7.7937E-03
200.0	5000.0	0.0500	3.8000E+00	7.9577E+00	1.1732E+00	1.8813E-02	9.8977E-03	3.8456E-05	7.7937E-03	3.8456E-05	7.7937E-03
200.0	10000.0	0.0005	3.8000E+00	7.9577E+00	1.1732E+00	3.7386E-02	1.9795E-02	7.6912E-05	1.5588E-02	7.6912E-05	1.5588E-02
200.0	10000.0	0.0050	3.8000E+00	7.9577E+00	1.1732E+00	3.7386E-02	1.9795E-02	7.6912E-05	1.5588E-02	7.6912E-05	1.5588E-02
200.0	10000.0	0.0500	3.8000E+00	7.9577E+00	1.1732E+00	3.7386E-02	1.9795E-02	7.6912E-05	1.5588E-02	7.6912E-05	1.5588E-02
200.0	50000.0	0.0005	3.8000E+00	7.9577E+00	1.1732E+00	1.7880E-01	9.8977E-02	3.8456E-04	7.7939E-02	3.8456E-04	7.7939E-02
200.0	50000.0	0.0050	3.8000E+00	7.9577E+00	1.1732E+00	1.7880E-01	9.8977E-02	3.8456E-04	7.7939E-02	3.8456E-04	7.7939E-02
200.0	50000.0	0.0500	3.8000E+00	7.9577E+00	1.1732E+00	1.7880E-01	9.8977E-02	3.8456E-04	7.7939E-02	3.8456E-04	7.7939E-02

TERMINAL VELOCITY = 7.8638E+01

-1.0: U .LT. UMF
-3.0: UB .LE. UMF/EMF

-2.0: U .GT. UT
-4.0: CONST .GT. 2, DELH .LT. 0

PROGRAM FLUIDBED3

This program is the same as FLUIDBED1, except in the specification of the perforated-plate gas distributor. Instead of specifying the number of perforations in the plate, two other parameters are specified: the radius of each perforation in the plate and the fraction of the plate area comprising the total perforation area. The program then calculates the number of holes in the plate. The new codes are:

PHR perforated plate hole radius (cm)

PVF fraction of plate area comprising total perforation area.

The code PRF is not valid. Program output is the same as for FLUIDBED1, except that an additional line is added, telling how many holes are in the perforated plate. A listing of FLUIDBED3 is given in Table E-6 followed by an example of program compilation and execution in Table E-7.

Table E-6. FLUIDBED3 listing.

```

1  PROGRAM FLUIDBED3(TAPE59)
2  REAL M,L,LMF
3  DIMENSION VALUE(9),NAME(11)
4  EQUIVALENCE (T,VALUE(1)),(P,VALUE(2)),(M,VALUE(3)),(HRAD,&
5  VALUE(4)),(RAD,VALUE(5)),(DP,VALUE(6)),(EMF,VALUE(7)),&
6  (CEWT,VALUE(8)),(EMPTY,VALUE(9))
7  DATA INAME,"TMP","PRS","BDS","PHR","RAD","DP","EMF",&
8  "GWT","PVF","RUN","END"/
9  COMMON /FLUID1/ L,LMF,UMF,UT,U,CIN,CDUT,CPPM1,CPPM0,DELP,&
10 POWER,DELTA
11 CALL CHANGE(4R*XY3)
12 T=EMF*M=DP*CEWT=HOLES=RAD=VALUER=HRAD=EMPTY=0.0
13 NAME=
14 C  ENTER DATA
15 1 WRITE(59,("/" " ENTER DATA""))
16 2 WRITE(59,(" " " ?""))
17 READ(59, "(A3,F20.10)")NAME,VALUER
18 DO 3 I=1,9
19 IF(NAME.NE.NAME(I))GO TO 3
20 IF(I.EQ.1)VALUER=VALUER*273.0
21 IF(I.EQ.6)VALUER=VALUER*1.0E-4
22 VALUE(I)=VALUER
23 GO TO 2
24 3 CONTINUE
25 IF(NAME.EQ.NAME(10))GO TO 4
26 IF(NAME.EQ.NAME(11))CALL EXIT
27 WRITE(59,(" " " INCORRECT ENTRY - " " ,A3)"")NAME
28 GO TO 2
29 4 DO 5 I=1,9
30 IF(VALUE(I).NE.0.0)GO TO 5
31 WRITE(59,(" " " " ,A3," " ?""))NAME(I)
32 GO TO 2
33 5 CONTINUE
34 HOLES=RAD*RAD=EMPTY/(HRAD=HRAD)
35 WRITE(59,(" " " VARY DELTA?""))
36 READ(59, "(A3)"")NAME
37 DELT=DP/2.0
38 DO 10 I=1,3
39 IF(NAME.NE."YES".AND.I.NE.2)GO TO 10
40 DELTA=DELT*10.0**(I-2)
41 CALL FLUID(T,P,M,HOLES,RAD,DP,EMF,CEWT)
42 C  OUTPUT DATA
43 WRITE(59,1000)CPPM1,CPPM0
44 FORMAT("/ " INLET CONC.= " ,E11.4," PPM      OUTLET CONC.= " ,E11.4," PPM")
45 WRITE(59,1001)U,UMF,UT
46 1001 FORMAT(" VELOCITIES: U= " ,E11.4," UMF= " ,E11.4," UT= " ,E11.4)
47 WRITE(59,1002)L,LMF
48 1002 FORMAT(" BED LENGTHS: L= " ,E11.4," LMF= " ,E11.4)
49 WRITE(59,1003)DELP,POWER
50 1003 FORMAT(" BED PRES. DROP OF " ,F8.3," ATM REQUIRES " ,E11.4,&
51 " KW POWER")
52 WRITE(59,1004)HOLES
53 1004 FORMAT(" DISTRIBUTOR PLATE HAS " ,E11.4," HOLES")
54 10 CONTINUE
55 GO TO 1
56 END

1  SUBROUTINE FLUID(T,P,M,HOLES,RAD,DP,EMF,CEWT)
2  REAL M,LMF,MU,K,L
3  COMMON /FLUID1/ L,LMF,UMF,UT,U,CIN,CDUT,CPPM1,CPPM0,DELP,&
4  POWER,DELTA
5  PI=3.141592654
6  RHOP=6.7
7  RHOGIN=40.0=P/(.82.057*T)
8  CPPM1=3.8
9  CIN=(RHOGIN/40.0)*CPPM1*1.0E-6
10 V=CEWT/(RHOP*(1.0-EMF))
11 A=RAD=RAD*PI
12 LMF=VMF/A
13 MU=17.78E-5*((4.58*T/151.-1.67)**0.625)*1.0E-2/0.02763
14 UHF=(SQRT(33.7*33.7+0.0408*DP*DP)*RHOGIN*(RHOP-RHOGIN))*&
15 980./(MU*MU))-33.7)*MU/(DP*RHOGIN)
16 UT=980.*DP*DP*(RHOP-RHOGIN)/(18.0*MU)
17 REP=DP*RHOGIN*UT/MU
18 IF(REP.LE.0.4)GO TO 10
19 UT=((4.0/225.0)*(RHOP-RHOGIN)*(RHOP-RHOGIN)*980.*980./&
20 (RHOGIN*MU))*((1.0/3.0)*DP
21 REP=DP*RHOGIN*UT/MU
22 IF(REP.LE.500.)GO TO 10
23 UT=(SQRT(18.0*980.0*(RHOP-RHOGIN)*DP/RHOGIN)
24 REP=DP*RHOGIN*UT/MU
25 IF(REP.LE.2.0E+05)GO TO 10

```

Table E-6. (Continued)

```

26 WRITE(59, "(" " UT?" " , 2E15.4) ") REP, UT
27 10 CONTINUE
28 F=1./OE7/(H=P)
29 U=1./A
30 DAB=1.524E-5*(T==1.823)/P
31 Q=(U-UMF)/HOLDS
32 IF(U.LT.UMF) GO TO 500
33 DO=(6.0*Q/P1)**0.4)/(980.0**0.2)
34 DB=DO
35 DBAR=1.4*RHOP*DP=(U/UMF)*(LMF/2.0)+DO
36 L=(U-UMF)/(0.711*SQRT(DBAR*980.0))*LMF+LMF
37 CONST=1.4*RHOP*DP=U/UMF
38 H=0.0
39 N=0
40 EPS=1.0-LMF*(1.0-EMF)/L
41 CBNM1=CIN
42 IF(U.GE.UT) GO TO 800
43 IF(CONST.GE.2.0) GO TO 800
44 100 N=N+1
45 DELHN=2.0*DO*((2.0+CONST)**(N-1))/((2.0-CONST)**N)
46 H=H+DELHN
47 IF(H.LT.LMF) GO TO 101
48 EPS=1.-(LMF*(1.0-EMF)/L)+LMF*(1.0-EMF)*(H-LMF)/(2.0*L*(L-LMF))
49 IF(EPS.GT.1.0) EPS=1.0
50 101 A=8.0*(1.0-EPS)/DP
51 K=DAB*AA/DELTA
52 UB=0.711*SQRT(DELHN*980.0)
53 IF(UB.LE.UMF/EMF) GO TO 700
54 CAPN=G.0*A*(L-LMF)/(P1*L*DELHN*DELHN)
55 CONST2=CAPN*P1*DELHN*DELHN*DELHN/(6.0*(UB-UMF/EMF))
56 VCN=CONST2*3.0*UMF/EMF
57 VBN=CONST2*(UB+2.0*UMF/EMF)
58 VEN=A*DELHN-VBN
59 IF(VEN.GE.0.0) GO TO 102
60 VEN=0.0
61 VBN=A*DELHN
62 102 CONTINUE
63 DB=CONST*H+DO
64 FONP=((1.0/DB)*(UB-UMF/EMF)/(UB+2.0*UMF/EMF)
65 CBN=(A*U*CBNM1)/(FONP*VBN*((1.0-FONP*VBN/(K*VEN+FONP*VBN))+&
66 K*VEN*A*U))
67 CEN=FONP*VBN*CBN/(K*VEN+FONP*VBN)
68 IF(H.GE.(LMF+2.0*(L-LMF))) GO TO 105
69 CBNM1=CBN
70 GO TO 100
71 105 COUT=CBN
72 CPPM0=CBN*1.0E+06/(RHOGIN/40.0)
73 WRITE(59, "(" " N = " , 110) ") N
74 GAMMA=1.8667
75 DELP=(1.0-EMF)*(RHOP-RHOGIN)*980.0*LMF*9.8692E-7
76 P2=P-DELP
77 IF(P2.GE.0) GO TO 106
78 POWER=-0.0
79 GO TO 110
80 106 POWER=-GAMMA/(GAMMA-1.0)*10.0E+6*((P2/P)**((GAMMA-1.0)/GAMMA))&
81 -1.0)*1.0E-3*74.74*0.0013558
82 110 CONTINUE
83 RETURN
84 CPPM0=L=LMF=DELP=POWER=-1.0
85 RETURN
86 CPPM0=L=LMF=DELP=POWER=-4.0
87 RETURN
88 CPPM0=L=LMF=DELP=POWER=-3.0
89 RETURN
90 CPPM0=L=LMF=DELP=POWER=-2.0
91 RETURN
92 END

```

Table E-7. FLUIDBED3 compilation and execution.

Compile and create controllee

```

CHAT FLUIDBED3 F360 F3BIN F3LIST Y02 M M / 1 1.4
LOADING
CODE BLOC      F360 WRITTEN
FILE SIZE=     0014332
FLD LGTH=      0014102    0012075

```

Execute controllee

```
F360 / 1 1
```

```

ENTER DATA
?
TMP 25.0
?
PRS 1.0
?
BDS 2.0
?
DPS 100.0
?
GWT 1000000.
?
EMF .4
?
RAD 250.0
?
PHR .3
?
RUN
PVF ?
?
PVF .1
?
RUN
VARY DELTA?
YES
N = 4

INLET CONC.= 3.8000E+00 PPM    OUTLET CONC.= 5.9026E-03 PPM
VELOCITIES: U= 2.5465E+01 LMF= 1.7689E+00 UT= 1.2783E+02
BED LENGTHS: L= 2.7139E+00 LMF= 1.2669E+00
BED PRES. DROP OF 0.005 ATM REQUIRES 4.9976E+00 KW POWER
DISTRIBUTOR PLATE HAS 6.9444E+04 HOLES
N = 4

INLET CONC.= 3.8000E+00 PPM    OUTLET CONC.= 5.8104E-02 PPM
VELOCITIES: U= 2.5465E+01 LMF= 1.7689E+00 UT= 1.2763E+02
BED LENGTHS: L= 2.7139E+00 LMF= 1.2669E+00
BED PRES. DROP OF 0.005 ATM REQUIRES 4.9976E+00 KW POWER
DISTRIBUTOR PLATE HAS 6.9444E+04 HOLES
N = 4

INLET CONC.= 3.8000E+00 PPM    OUTLET CONC.= 5.0259E-01 PPM
VELOCITIES: U= 2.5465E+01 LMF= 1.7689E+00 UT= 1.2763E+02
BED LENGTHS: L= 2.7139E+00 LMF= 1.2669E+00
BED PRES. DROP OF 0.005 ATM REQUIRES 4.9976E+00 KW POWER
DISTRIBUTOR PLATE HAS 6.9444E+04 HOLES

ENTER DATA
?

ALL DONE

```

Appendix F: Heat Effects of Gettering Reaction

From Table 1 in the main text of this report, the heat reaction is:

There are 21.6 g of tritium to be gettered. Assuming the heat of reaction is the same for hydrogen and tritium, the heat of reaction at 25°C becomes:

$$Q = \frac{21.6 \text{ g T}_2}{6 \text{ g T}_2/\text{mol T}_2} \times -206 \frac{\text{kJ}}{\text{mol T}_2} = -742 \text{ kJ}.$$

Therefore, for adiabatic operation (which gives the largest temperature increase of the solid), the cerium must absorb 742 kJ.

The specific heat of cerium at 25°C is 192 J/kg°C (from Table 1). Therefore, for mass of cerium GWT,

$$(\text{GWT})\text{kg}(192) \frac{\text{J}}{\text{kg}^\circ\text{C}} \Delta T = 742 \text{ kJ} \times \frac{10^3 \text{ J}}{\text{kJ}} \quad (\text{F-1})$$

$$\Delta T = \frac{3.86 \times 10^3}{\text{GWT}} ^\circ\text{C}. \quad (\text{F-2})$$

For the fixed bed, GWT = 650 kg and $\Delta T = 5.9^\circ\text{C}$.

For the fluidized bed, GWT = 2000 kg and $\Delta T = 1.9^\circ\text{C}$.

Thus, even for adiabatic operation, both reactors are almost isothermal. Since actual operation is unlikely to be adiabatic (some heat will be removed in the gas), both reactors will be essentially isothermal in operation.