Heat Transfer Calculations For Normal Operations Of A Fixed CST Bed Column

Si Young Lee

SAFETY · RESPONSIBILITY · SECURITY

SRS

SAVANNAH RIVER SITE

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-96SR18500 with the U.S. Department of Energy.

DISCLAIMER

Heat Transfer Calculations For Normal Operations Of A Fixed CST Bed Column

SAVANNAH RIVER TECHNOLOGY CENTER

Si Young Lee

(This Page Intentionally Left Blank)

DOCUMENT: WSRC-TR-2001-00255
TITLE: Heat Transfer Calculations For Normal Operations Of A Fixed CST Bed Column

APPROVALS

_____   Date:_____
Si Y. Lee, Author (EM&S Group/ SRTC)

_____   Date:_____
Richard A. Dimenna, Technical Review (EM&S Group/ SRTC)

_____   Date:_____
Jeff A. Pike, Customer (HLW Process Engineering)

_____   Date:_____
Richard E. Edwards, Jr., Manager (HLW Process Engineering)

_____   Date:_____
Joe T. Carter, Director of Engineering (Salt Waste Disposition Facility)

_____   Date:_____
Dennis W. Wester, TFA CST System Lead (Pacific Northwest National Laboratory)

_____   Date:_____
Cynthia P. Holding-Smith, Manager (EM&S Group/SRTC)

_____   Date:_____
Steve T. Wach, Manager (EDS/SRTC)

(This Page Intentionally Left Blank)

Table of Contents

(This Page Intentionally Left Blank)

List of Figures

List of Tables

Nomenclature

a_p = surface area of a single particle (m^2)

A = total surface area (m^2)

C_p = specific heat (J/kgK)

d = diameter (m)

g = gravity (m/sec^2)

h = enthalpy (J/kg) or heat transfer coefficient (W/m^{2}K)

k = thermal conductivity (W/mK)

H = column height or characteristic length (m)

n = total number of particles contained in the column

Nu = Nusselt number, hd/k

Pr = Prandtl number, $\mu C_p/k$

q'' = heat flux (W/m^2)

q''' = heat generation source per unit volume (W/m^3)

Q_h = heat transfer rate (W)

r = radial distance from the center of CST column (m)

R = column radius (m)

Re = Reynolds number, $d\rho u/\mu$

T = temperature (^{o}C)

u = superficial velocity in porous media (m/sec)

v = local interstitial velocity (m/sec)

V = volume (m^3)

x = local position along the x-direction under Cartesian coordinate system

y = local position along the y-direction under Cartesian coordinate system

z = vertical position along the bulk flow direction

Greek

α = particle surface area per unit volume (m^{-1})

ρ = density (kg/m^3)

Δ = difference

μ = dynamic viscosity (N sec/m^2)

ν = kinematic viscosity (m^2/sec)

Subscript

avg = average

Bed = bed

eff = effective

exit = column exit

f = bulk fluid

i = initial or interface

inlet = column inlet

m = center of a single particle in a fully-loaded CST column

max = maximum

p = particle

s = surface of a solid particle

w or wall = column wall

∞ = ambient

WESTINGHOUSE SAVANNAH RIVER COMPANY

HEAT TRANSFER CALCULATIONS FOR NORMAL

OPERATIONS OF A FIXED BED COLUMN

Report:WSRC-TR-2001-00255

Date: 07/24/01

Page: 1 of 24

Abstract

In support of the crystalline silicotitanate (CST) ion exchange project of High-Level Waste (HLW) Process Engineering, heat transfer calculations have been made for a fully-loaded CST column during abnormal and normal operating conditions.

The modeling and calculations have been performed using theoretical and computational heat transfer approaches. The previous heat transfer calculations [Ref. 1] estimated conservative heat transfer rates for the column under no-flow conditions. For the present analysis, three basic cases were theoretically considered to estimate sensitivities of temperature distributions with respect to the configurations of fluid-particle systems. Steady-state temperature responses to a uniform heat source in a fixed bed were estimated using the literature data. A theoretical, one-dimensional approach was taken by considering overall energy balance for the CST column. A computational heat transfer approach was also taken to estimate detailed flow distribution effects on the temperature profiles of a fixed bed CST column. In this approach, the commercial finite volume code, CFX [Ref. 4], was used to create a prototypic geometry file under a non-orthogonal mesh environment. In this case, a node-mapping technique was developed to consider convection effect in the energy equation due to the fluid motion in porous media with a heat source present in the solid particle region.

All the analysis results demonstrate that about 21gpm process flow of the normally operating CST column provides adequate heat removal from a fully-loaded fixed bed column containing 94 W/ft^3 heat source. The results of a single particle model show that there are negligible temperature differences between the center and surface of a single solid particle for the conditions considered here. From the analysis of fluid-particle systems, the temperature gradient at the particle-fluid interface of a loosely-packed bed is found to be much lower than that of a packed bed from the experimental data available in the literature. For the normal flow conditions of a fixed CST bed, average temperature difference between the particle surface and the bulk fluid medium is found to be less than 0.5^{o}C.

The theoretical and simulation results show that about 30°C of average fluid temperature is reached at the exit plane of the column when a fully-loaded CST column has a 94 W/ft^3 heat source and a 25°C inlet temperature under the normal flow condition. The simulation results show that a maximum local temperature of about 34°C is reached at the exit of the bed column. In this case, the fluid temperature is about 1°C lower than the particle temperature for the operating conditions of the CST column when the column wall is cooled by natural convection.

From the sensitivity study of the CST design parameters, it was found that whether the column is loosely-packed or densely-packed is a key parameter associated with the coolability of a fully-loaded CST column under normal flow conditions since bed porosity is closely related to the effective energy transport of the column. In addition, the results computed by the simulation model were verified by the theoretical results.

The analysis results will provide quantitative information associated with the process heat control and management of the CST column base design.

1. Introduction

The crystalline silicotitanate (CST) ion exchange process treats high-level radioactive waste for feed to the saltstone facility to be made into grout. Through this process, radionuclides such as strontium, plutonium, and uranium are removed by the monosodium titanate (MST) addition, and then cesium nuclide from the salt supernate solution is absorbed into the CST bed.

An ion exchange column loaded with the CST will generate significant heat from radioactive decay. The CST material in the bed column is being used as an inorganic ion-exchange media to remove cesium nuclide from the supernatant stored in the high-level radioactive waste tanks at the Savannah River Site (SRS). The supernatant is primarily a mixture of aqueous sodium nitrate and sodium hydroxide with smaller concentrations of other species. Sorption of the cesium from the supernatant results in concentrating the cesium into the volume of the CST. In this situation, the cesium becomes a source of significant thermal energy in the column.

If engineering designs of the CST sorption column can not handle this thermal load, hot spots may develop locally within the column and degrade the performance of the ion-exchange process. Thus, heat transfer analyses for a fully-loaded CST column have been performed for transient no-flow and steady-state normal operation conditions as shown in Table 1. In the previous calculations [Ref. 1], a conservative approach was taken. That is, a conduction-dominant cooling mode was considered for loss of flow or no flow conditions through the CST column assuming convection effect to be negligible. The previous report presented transient thermal responses to no-flow conditions of a fully-loaded CST column for various modeling boundary and design conditions.

The objective of the present work is to compute temperature distributions across the column when there is steady flow of salt solution through the CST column under normal conditions of the process operations. In this situation, the High-Level Waste (HLW) customer [Ref. 2] requested that the calculations should be conservative in that the model results would show the maximum temperatures achievable by the CST design configurations under normal flow conditions. Schematic diagram for the CST column system is illustrated in Fig. 1.

The analysis results will be used to evaluate the fluid temperature distributions and the process component temperatures within the ion exchange system. This information will also assist in the system base design.

Table 1. Status of heat transfer analysis for a fixed porous bed of a fully-loaded CST column.

System Conditions	Modeling Approaches	Doc. of Analysis Results
Loss of process flow	Transient analysis for no-flow conditions	Done [Ref. 1]
Normal operations	Steady-state analysis for 21gpm normal flow	Present analysis

WESTINGHOUSE SAVANNAH RIVER COMPANY

HEAT TRANSFER CALCULATIONS FOR NORMAL
OPERATIONS OF A FIXED BED COLUMN

Report:WSRC-TR-2001-00255
Date: 07/24/01

Page: 3 of 24

2. Modeling Approach and Analysis

For the CST operation, the column bed requires the dimensions of 16 ft long and 5 ft diameter to maintain the designed process rates. A fully-loaded column may generate as much as about 6×10^6 Ci radioactivity. This highly concentrated radioactive source will contain a significant amount of heat load in the column, which corresponds to about 94 W/ft^3 of volumetric heat source based on total volume of the bed.

The results of the present analysis will determine if process fluid flow through the column under normal operating conditions provides adequate heat removal from a fully-loaded fixed bed CST column containing the decay heat source. Detailed reference design and normal operating conditions are shown in Table 2. Under this normal flow situation of the CST column, there are some concerns about what is maximum local temperature difference between the CST particle and its surrounding fluid for the steady-state normal flow conditions of the fully-loaded column and how effectively the column cools down along the axial flow direction under the current design configurations.

Process flow

u_f

$z = 0$ (bed inlet), T_{inlet}

z

$T(z)$

Packed bed column region
(heat source region)
q'''

A ――――――― A'

$z = H_{Bed}$
(bed exit), T_{exit}

u_f

Column height: 16 ft
Column diameter: 5 ft
Particle size = 500 or 700 microns
Porosity = about 40%
q''' = 94 W/ft^3

SS wall (0.5 inches)

h_{wall}

T_∞

CST bed
(60-inch diameter)

0

$T_f(r)$

q'''

r

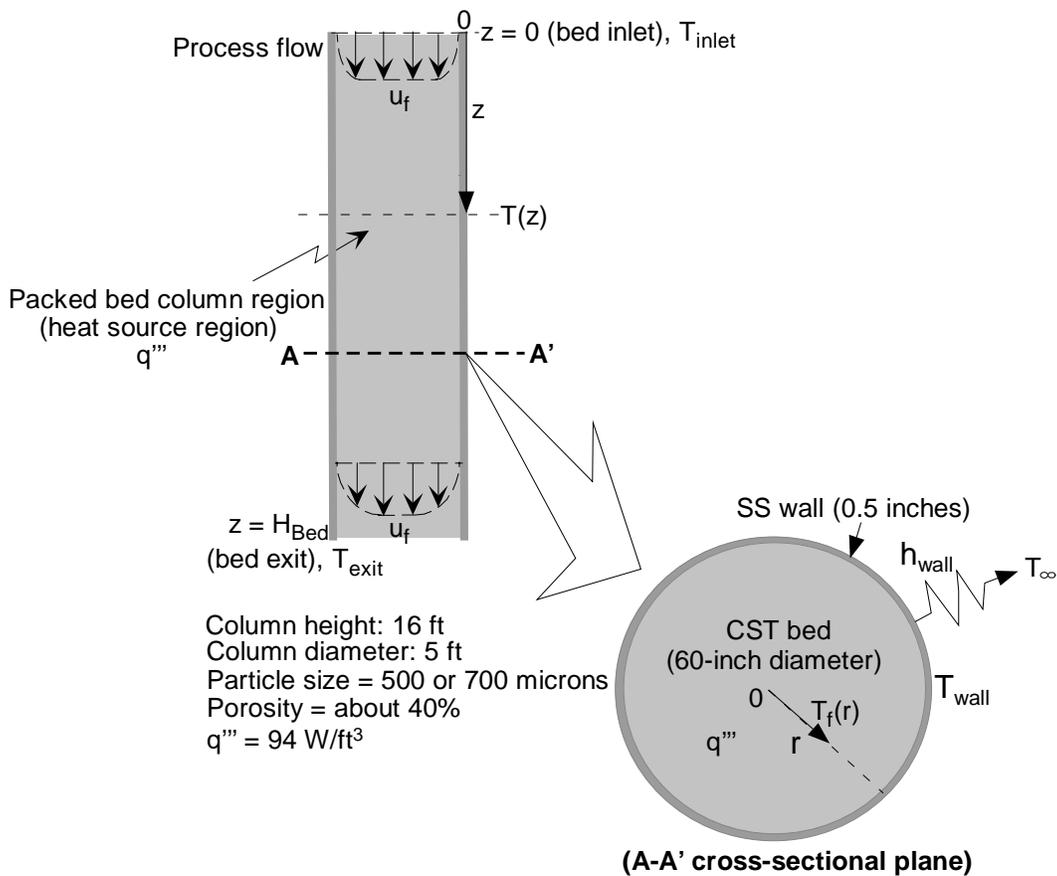T_{wall}

(A-A' cross-sectional plane)

Figure 1. Schematic illustrations of CST packed bed column under normal flow conditions

For the present analysis, theoretical and computational approaches were taken to calculate temperature distributions for the modeling domain of the CST column using the literature data. In this case, one-dimensional steady-state overall energy balance for the column domain was considered to calculate temperature profiles for the particle-fluid systems. A three-dimensional computational fluid dynamics (CFD) approach was taken to examine the non-uniform flow effect on local temperature distributions of a fully-loaded CST column. In this approach, the commercial finite volume code, CFX [4], was used to create prototypic geometry file under non-orthogonal mesh environment.

The analysis consists of two major parts as presented in Table 3. One part is to estimate maximum temperature difference between the center and surface of a single particle assuming that every CST particle has perfectly spherical shape with uniform volumetric heat source. The second part is to perform heat transfer analysis for the fluid-particle system in a porous bed after evaluating the internal temperature gradient for a single CST particle with heat generation source from the first part. In the second part of the analysis, the model considers three basic cases with different boundary conditions to investigate how sensitive the temperature profiles for porous bed with uniform heat source are to various conditions of the particle-fluid system in a porous bed.

The CST column system to be analyzed here is illustrated in Fig. 1. The model geometry was created using the body-fitted coordinate system and structured multi-block grids in the CFD preprocessing environment. For the heat transfer analysis, the reference design conditions were considered as shown in Table 2. Spherical CST particles (about 500-micron or 700-micron diameter) are packed inside a column of stainless steel cylinder that is 16 ft high and 5 ft diameter along the 0.5-inch thick wall. In the present analysis, the resistance of heat transfer across the column wall was neglected from the previous results [Ref. 1]. The porosity of the CST packed bed was assumed to be about 40 % for conservative estimations of temperature profiles within the column although the porosity the customer provided [Ref. 2] was higher than 40%. In the ORNL work, the density of the salt solution was estimated to be about 1255 kg/m^3 considering that density of CST solid is 2,056 kg/m^3. Thermal conductivity of the solution was used as 0.15538 W/mK (evaluated at 25°C temperature). Detailed material and thermal properties used in the analysis are shown in Table 4.

2. 1 Temperature distributions inside spherical solid particle with heat generation source

Internal temperature distributions of a single solid particle can be calculated theoretically for uniformly distributed heat source. Steady-state governing equation for the conduction-controlled solid medium with uniform volumetric heat source q''', as shown in Fig. 2, can be written under spherical coordinate system as

$$\frac{1}{r^2}\left(\frac{d}{dr}r^2\frac{dT(r)}{dr}\right) + \frac{q'''}{k_f} = 0 \tag{1}$$

where k_f is thermal conductivity of the solid sphere.

Table 2. Reference design conditions used for the present analysis.

Parameters	Conditions
Bed column dimensions (d_{Bed} x H_{Bed})	5ft diameter x 16ft high
Particle diameter (d_p)	500* and 700 microns
Bed porosity (ε)	0.40**
Salt solution temperature at inlet (T_{inlet})	25^oC
Salt solution flowrate	21 gpm
Superficial fluid velocity (u)	7.26×10^{-4} m/sec
Heat generation rate per bed volume (q'''_{Bed})	94 W/ft^3 (=3319.6 W/m^3)

Note: *500-micron particle is used for the normal operation analysis of a
      fully-loaded CST column.
      **40% porosity (instead of 50%) is used for a conservative approach

Table 3. Modeling approaches taken for the present analysis.

Analysis Domain	Analysis Cases	Modeling Approaches	Primary Purposes
Single Solid Particle	---	Theoretical	To estimate maximum temperature difference for a single particle domain containing heat source
Particle-Fluid System	Case-I	Theoretical	To evaluate heat transfer for a single sphere containing heat source in stagnant bulk fluid (simulated as loosely-packed bed)
	Case-II	Theoretical	To evaluate heat transfer for a single sphere containing heat source in a flowing fluid (simulated as a loosely-packed bed)
	Case-III	Theoretical	To estimate heat transfer capability for a closely-packed and fixed bed in a flowing fluid using one-dimensional energy transport
		Numerical (CFD)	To estimate heat transfer capability for a fixed fully-loaded CST column in a flowing fluid using multi-dimensional momentum and energy transport

Equation (1) is imposed by the boundary conditions at the center of the sphere (r = 0).

$$T(r = 0) = T_m \quad \text{and} \quad \left.\frac{dT}{dr}\right|_{r=0} = 0 \tag{2}$$

Spatial temperature distributions within the solid region of spherical particle can be determined by using eqs. (1) and (2) in terms of heat generation rate per particle volume (q''') and thermal conductivity of the particle.

$$T(r) = T_m - \left(\frac{q'''}{6k_p}\right)r^2 \tag{3}$$

Maximum temperature difference between the center and surface of spherical solid can be obtained in terms of volumetric heat source as

$$(T_m - T_s) = \left(\frac{q'''}{24k_p}\right)(d_p)^2 . \tag{4}$$

Mathematical notations used in eq. (4) are described in Fig. 2.

When bed porosity and particle surface temperature are assumed to be uniform, maximum temperature difference between the center and surface of spherical solid can be obtained in terms of volumetric heat source based on bed volume (q_{Bed}''') as

$$(T_m - T_s) = \left(\frac{q_{Bed}'''}{24k_p(1-\varepsilon)}\right)(d_p)^2 . \tag{4a}$$

r_p = radius of particle
k_p = thermal conductivity of particle
T_m = temperature at the center of particle (r = 0)
T_s = temperature at the surface of particle (r = r_p)
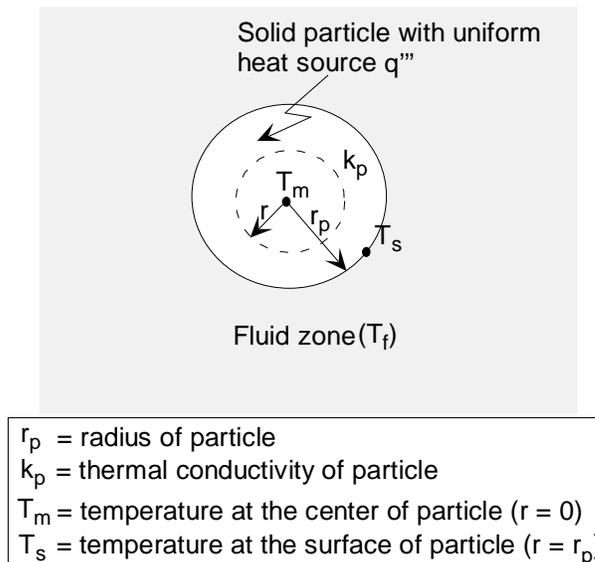
Figure 2. Heat transfer for a single particle with volumetric heat source q'''

WESTINGHOUSE SAVANNAH RIVER COMPANY   Report:WSRC-TR-2001-00255
Date: 07/24/01
HEAT TRANSFER CALCULATIONS FOR NORMAL
OPERATIONS OF A FIXED BED COLUMN   Page: 7 of 24

2.2 Heat Transfer Analysis for Fluid-Particle System in Porous Bed

2.2.1 Heat Transfer between Stagnant Fluids and Single Particle (Case-I)

Transfer of heat from sphere to the stagnant surrounding medium has been treated by conduction theoretically as shown in Fig. 3. Rudenberg (1925) showed that the exchange rate Q_h of heat by conduction between a sphere acting as a heat source and its surroundings can be represented by the relation

$$Q_h = 2\pi d_p k_f \left(1 + \frac{d_p}{4z}\right)^{-1} (T_s - T_f) \tag{5}$$

In eq. (5) T_s represents the surface temperature of a spherical particle and T_f the temperature of the surroundings measured at large distance z from the spherical solid relative to the diameter of the sphere (d_p). k_f is thermal conductivity of the surrounding fluid in eq. (5). In terms of the conventional heat transfer coefficient h_f defined by the relation

$$Q_h = h_f a_p (T_s - T_f) = (\pi d_p^2) h_f (T_s - T_f) \tag{6}$$

When z is much larger than d_p, eq. (5) becomes

$$Q_h = 2\pi d_p k_f (T_s - T_f) \tag{7}$$

From the comparison between eq. (6) and eq. (7), Nusselt number can be obtained in terms of spherical diameter d_p.

$$Nu = \frac{d_p h_f}{k_f} = 2 \tag{8}$$

When CST particle size is 500 microns, heat transfer coefficient h_f at the surface of the CST particle is calculated as 2720 W/m^{2}K for thermal conductivity of the salt solution provided in Table 4. In this case temperature difference between the surface of particle and stagnant bulk fluid can be computed by eq. (9) for given particle size and volumetric heat source of the bed column.

$$(T_s - T_f) = \frac{Q_h}{h_f a_p} = \frac{q_{Bed}'''}{h_f \alpha_p (1 - \varepsilon)} \tag{9}$$

In eq. (9) the ratio α_p of the area to volume of a single particle becomes

$$\alpha_p = \frac{a_p}{V_p} = \frac{6}{d_p} \tag{10}$$

Report: WSRC-TR-2001-00255
Date: 07/24/01

Page: 8 of 24

WESTINGHOUSE SAVANNAH RIVER COMPANY

HEAT TRANSFER CALCULATIONS FOR NORMAL
OPERATIONS OF A FIXED CST BED COLUMN
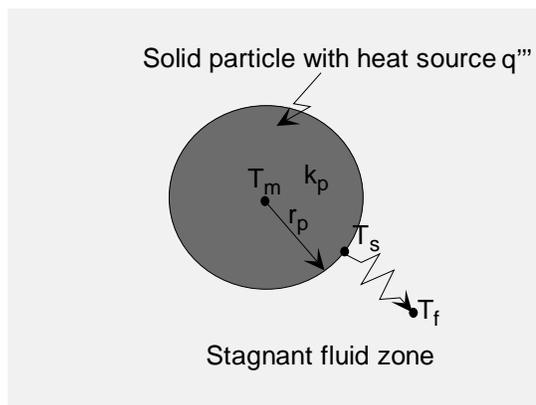
Figure 3. Heat transfer for a single particle with heat generation in stagnant liquid medium (Case-I)

Table 4. Material, thermal, and transport properties for the CST column heat transfer calculations.

Material	Thermal conductivity (W/mK)	pecific heat (J/kgK)	Density (kg/m3)	Viscosity (cp)
CST [Ref. 2]	$0.13968+6.2800 \times 10^{-4} T^*$	1052.3	2056.3	---
Salt Solution [Ref. 2]	0.68	3630.0	1255.4	2.0**
Stainless steel [Ref. 17]	17.30	486.0	7800.0	---

Note: * T in ^{o}C (evaluated at 25°C temperature)
      ** Ref. 10

2.2.2 Heat Transfer of a Single Particle under Forced Convection Cooling (Case-II)

Forced convection heat transfer for a single sphere submerged in moving fluids can be evaluated by using empirical correlation available in the literature. This case is also designed to simulate the heat transfer of particles in loosely-packed bed or dilute suspension systems. The situation is illustrated in Fig. 4. Forced convection heat transfer for this situation is given by the literature [Kramers, 1946].

$$Nu = 2.0 + 1.3\,Pr^{0.15} + 0.66\,Pr^{0.31}\,Re_p^{0.5} \qquad (11)$$

In eq. (11) Reynolds number (Re_p) is evaluated in term of particle diameter (d_p) and superficial fluid velocity (u_f).

$$Re_p = \frac{\rho_f d_p u_f}{\mu_f} \qquad (12)$$

For the present 21 gpm flow condition and 500-micron particle size, the Reynolds number (Re_p) is about 0.23. In this situation, heat transfer coefficient h_f is computed by

eq. (11) using material and thermal properties given in Table 4. That is, h_f = 6138.9 (W/m²K). In this case temperature drop across the interface of particle surface and flowing fluid can calculated by eq. (9).
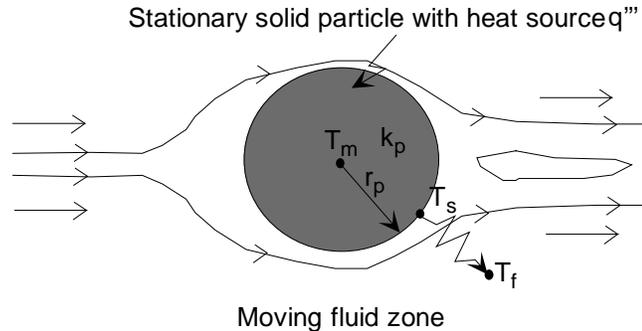
Figure 4. Heat transfer for a fixed single particle with heat generation source in moving fluid (Case-II)

2.2.3 Particle-Fluid Heat Transfer for Fixed CST Bed under Forced Convection (Case-III)

The heat transfer between beds of particles and fluid flowing through the interstices is evaluated for steady-state normal operating conditions of the CST bed column as shown in Fig. 5. Heat source per bed volume is about 3319.6 W/m³, which is equivalent to 94 W/ft³. For normal operating conditions, superficial velocity is about 0.7 mm/sec corresponding to 21 gpm flow in 5ft diameter CST column. In this situation the Reynolds number is about 0.23 for 500 micron particle diameter. Gunn and Souza (1974) made a collection of experimental results of the particle Nusselt number group at low Reynolds numbers. Nusselt number estimated by their empirical results was used for the present analysis. That is, particle Nusselt number (Nu) was found to be about 0.001, resulting in h_f = 1.36 W/m²K for the present conditions. Temperature difference between the particle surface and its surrounding fluid was computed by the conventional heat transfer relation.

$$
\begin{aligned}
(\varDelta T)_{Bed} &= (T_s - T_f)_{Bed} = \left(\frac{Q_h}{h_f A_p} \right) \\
&= \frac{1}{h_f} \left(\frac{V_{Bed}}{A_p} \right) q_{Bed}''' = \frac{q_{Bed}'''}{h_f \alpha_{Bed}}
\end{aligned}
\tag{13}
$$

In eq. (13) the ratio (α_{Bed}) of total particle surface area (A_p) to bed volume (V_{Bed}) is required to calculate the temperature difference ($(\varDelta T)_{Bed}$) across the interface of particle-fluid in a packed bed. When bed porosity (ε) is known, total volume of particles contained in a bed column (V_p) can be found from the bed volume.

$$
V_p = (1-\varepsilon)V_{Bed}
\tag{14}
$$

This particle volume can be used to compute total number of particle (n) contained in the bed corresponding to total volume of the particle.

Report: WSRC-TR-2001-00255
Date: 07/24/01

Page: 10 of 24

WESTINGHOUSE SAVANNAH RIVER COMPANY

HEAT TRANSFER CALCULATIONS FOR NORMAL
OPERATIONS OF A FIXED CST BED COLUMN

$$n = \frac{6 V_{Bed}(1-\varepsilon)}{\pi d_p^{\,2}}$$

(14a)

From eq. (14a) total surface area of the spherical particles in the bed (A_p) can be computed. That is

$$A_p = n\left(\pi d_p^{\,2}\right)$$

(14b)

From eqs. (14a) and (14b), ratio of the total heat transfer area of the particles to the volume of the bed can be calculated as

$$\alpha_{Bed} = \left(\frac{A_p}{V_{Bed}}\right) = \frac{6(1-\varepsilon)}{d_p}$$

(14c)
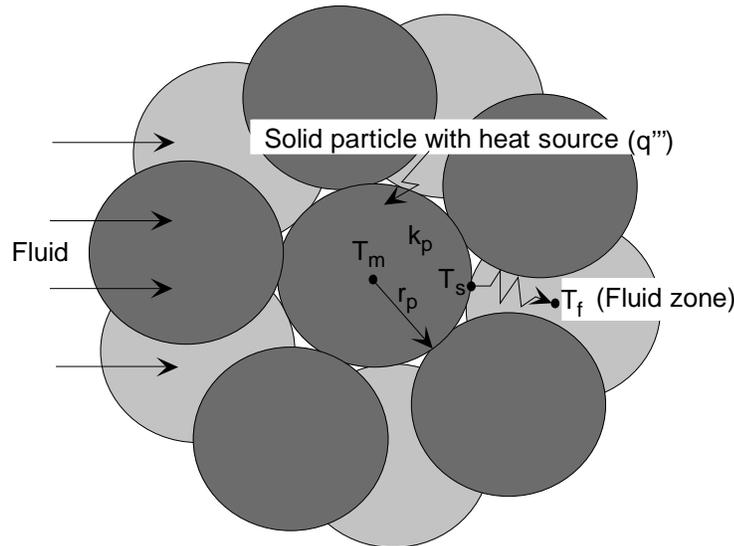
Figure 5. Heat transfer for a fixed porous bed with heat generation source under forced convection cooling condition (Case-III)

2.2.4 CFD Approach for Heat Transfer Analysis for CST Column (Case-III)

A computational heat transfer approach was taken to examine multi-dimensional flow distribution effect on fluid and particle surface temperatures and to compare the results with theoretical predictions. For the present analysis, CFX code was used as a computational fluid dynamics (CFD) tool. In the CFD simulations, packed bed is modeled as porous region. The solid portion of the packed bed, which is occupied by the particles, restricts the volume available to the fluid and also offers a resistance resulting in a higher pressure drop. This is modeled by specifying a volume porosity and resistance for the porous region. In the current CFD code, this approach does not

WESTINGHOUSE SAVANNAH RIVER COMPANY Report:WSRC-TR-2001-00255
               Date: 07/24/01
HEAT TRANSFER CALCULATIONS FOR NORMAL
OPERATIONS OF A FIXED BED COLUMN   Page: 11 of 24

model the solid portion of the bed, which has heat generation source. The code was modified by user-fortran programs to make energy coupling between fluid and solid cells. A mesh-mapping technique was used to allow energy exchange between the computational cells for the fluid and solid zones.

The main assumptions made regarding the present modeling assessment of heat transfer of the CST column are given as follows:

- The bed is maintained at a steady state with 21 gpm flowrate and is assumed to behave as a volumetrically heated porous medium.

- The bed consists of uniform size and spherical particle.

- There is no flow blockage within the porous flow medium.

- The mean value of bed porosity is equal to the local value in a bed.

- The fractional area of the bed occupied by channeling is assumed to be negligible, which is appropriate for a deep bed (16 ft deep for the CST column)

- Thermal and transport properties of the component materials are assumed to be constant for the present operating conditions.

- Radiation heat transfer is assumed to be negligible compared to convection because of low operation temperature (about 25°C).

The geometry to be modeled here is a cylindrical container of 5ft diameter as shown in Fig. 6. To model the solid region of the bed, the porous region is duplicated. The duplicated region is placed separated from the main problem as shown in Fig. 6. This region is defined as a conducting solid and is coupled to the fluid passing through the porous region by using user-fortran routines for heat transfer purposes. Three-dimensional non-uniform meshes for the computational domain are shown in Fig. 7. A heat transfer coefficient available in the literature was used for the estimation of the particle-to-fluid heat transfer rate. In the calculation, a heat transfer coefficient of 1.36 W/m^{2}K (equivalent to Nu = 0.001) was used. Optimum number of computational meshes is about 42,000. Reynolds number for the present analysis is about 0.23 based on the operating conditions shown in Table 2, hence a laminar flow calculation is performed.

For theoretical calculations of the axial heat transfer through a fixed bed, one-dimensional integral approach was used assuming that CST particles are homogeneously distributed through a fixed bed and heat is generated uniformly along the flow direction. The heat transfer at the wall of the CST column is assumed to be adiabatic to make one-dimensional approach valid. When there is uniform volumetric heat source (q''') for porous bed as shown in Fig. 8, one-dimensional steady-state integral energy balance along the axial flow z-direction through a bed becomes

$$A_{Bed}C_{pf}\int_{T_f=T_{iinlet}}^{T_f=T_{exit}}\left(\rho_f u_f\right)dT_f(z) = q_{Bed}''' A_{Bed}\int_{z=0}^{z=H_{Bed}} dz \qquad (15)$$

In eq. (15) A_{Bed} and H_{Bed} are superficial flow area and height of the CST column, respectively. C_{pf} in eq. (15) is specific heat of process fluid. When fluid is assumed to be incompressible, the temperature difference between the exit and the inlet of the bed can be estimated by eq. (15).

Report: WSRC-TR-2001-00255
Date: 07/24/01

Page: 12 of 24

WESTINGHOUSE SAVANNAH RIVER COMPANY

HEAT TRANSFER CALCULATIONS FOR NORMAL
OPERATIONS OF A FIXED CST BED COLUMN

$$\left(T_f(z) - T_{inlet}\right) = \left(\frac{q'''}{\rho_f u_{avg} C_{pf}}\right) z \tag{16}$$

u_{avg} in eq. (16) represents fluid velocity averaged over the flow area based on empty column at each elevation. That is

$$u_{avg} = \frac{1}{A_{Bed}} \int_{r=0}^{r=R_{Bed}} 2\pi r u(r)\, dr \tag{17}$$

In eq. (17) local interstitial velocity $v(r)$ is related to superficial velocity $u(r)$ in terms of porosity ε.

$$v(r) = \left(\frac{u(r)}{\varepsilon}\right) \tag{18}$$

For an incompressible flow with constant flow area, average superficial velocity (u_{avg}) under steady-state flow condition is constant along the z-direction shown in Fig. 8. For given particle size and volumetric heat source, maximum particle temperature at the exit of the CST column can be obtained in terms of fluid velocity and heat transfer coefficient. After some algebraic rearrangements of eqs. (4a), (13), and (16), maximum particle temperature at the exit of the column becomes

$$\{T_m - T_{inlet}\}_{exit} = (T_m - T_s)_{exit} + (T_s - T_f)_{exit} + \{T(z = H_{Bed}) - T_{inlet}\}$$

$$\approx \left(\frac{d_p^{\,2}}{24 k_p(1-\varepsilon)} + \frac{d_p}{6 h_f(1-\varepsilon)} + \frac{H_{Bed}}{\rho_f u_{avg} C_{pf}}\right) q_{Bed}''' \tag{19}$$

The above equation for maximum bed temperature is based on a one-dimensional concept. It shows that maximum particle temperature occurs at the exit plane of the column. Note that maximum temperature of the CST bed increases because of the reduced convection energy transport as process fluid velocity of the column decreases during normal operating conditions.

WESTINGHOUSE SAVANNAH RIVER COMPANY

HEAT TRANSFER CALCULATIONS FOR NORMAL
OPERATIONS OF A FIXED BED COLUMN

Report:WSRC-TR-2001-00255
Date: 07/24/01

Page: 13 of 24
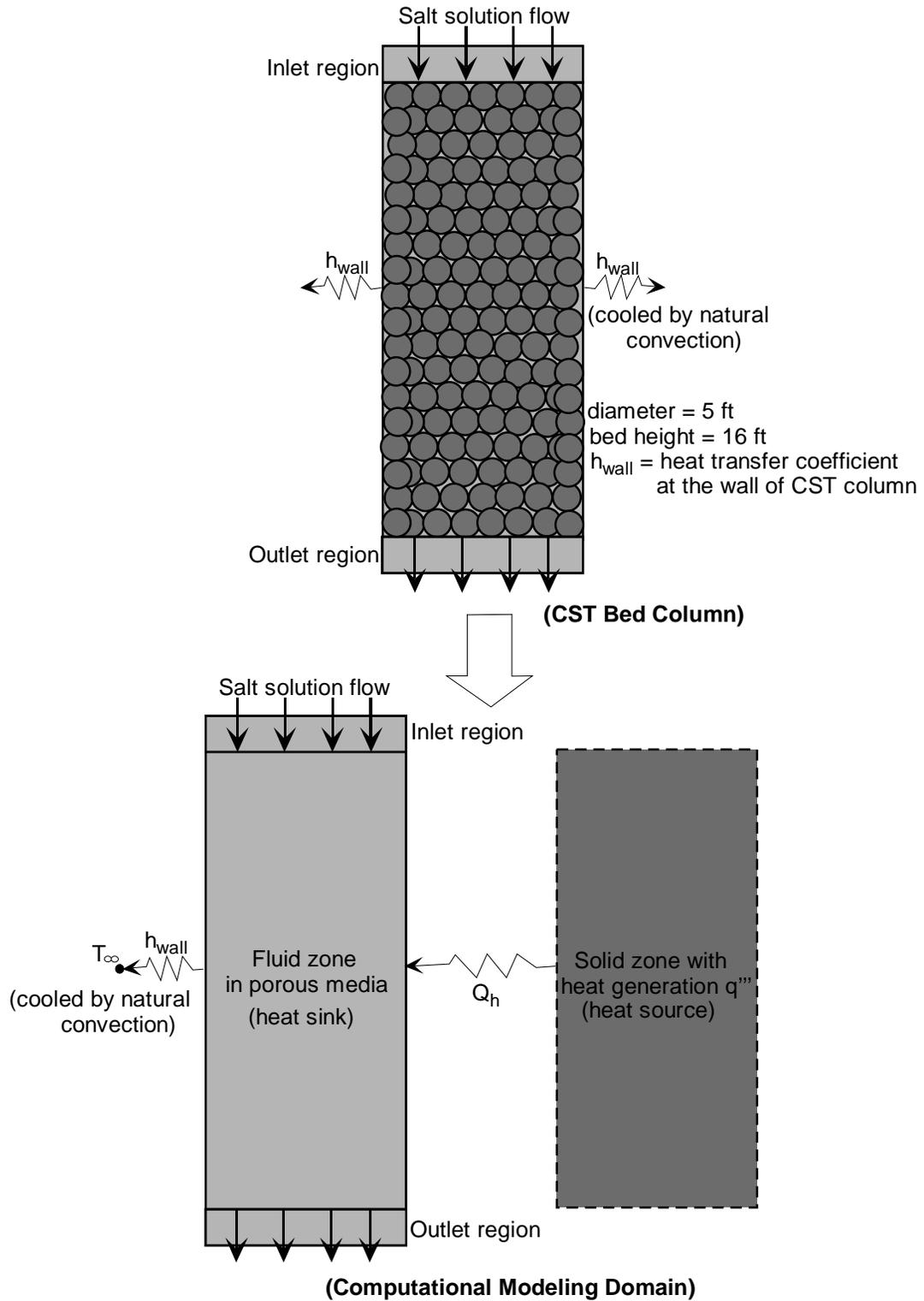
Figure 6. Computational model for the heat transfer in CST column using CFD approach.

WESTINGHOUSE SAVANNAH RIVER COMPANY

HEAT TRANSFER CALCULATIONS FOR NORMAL
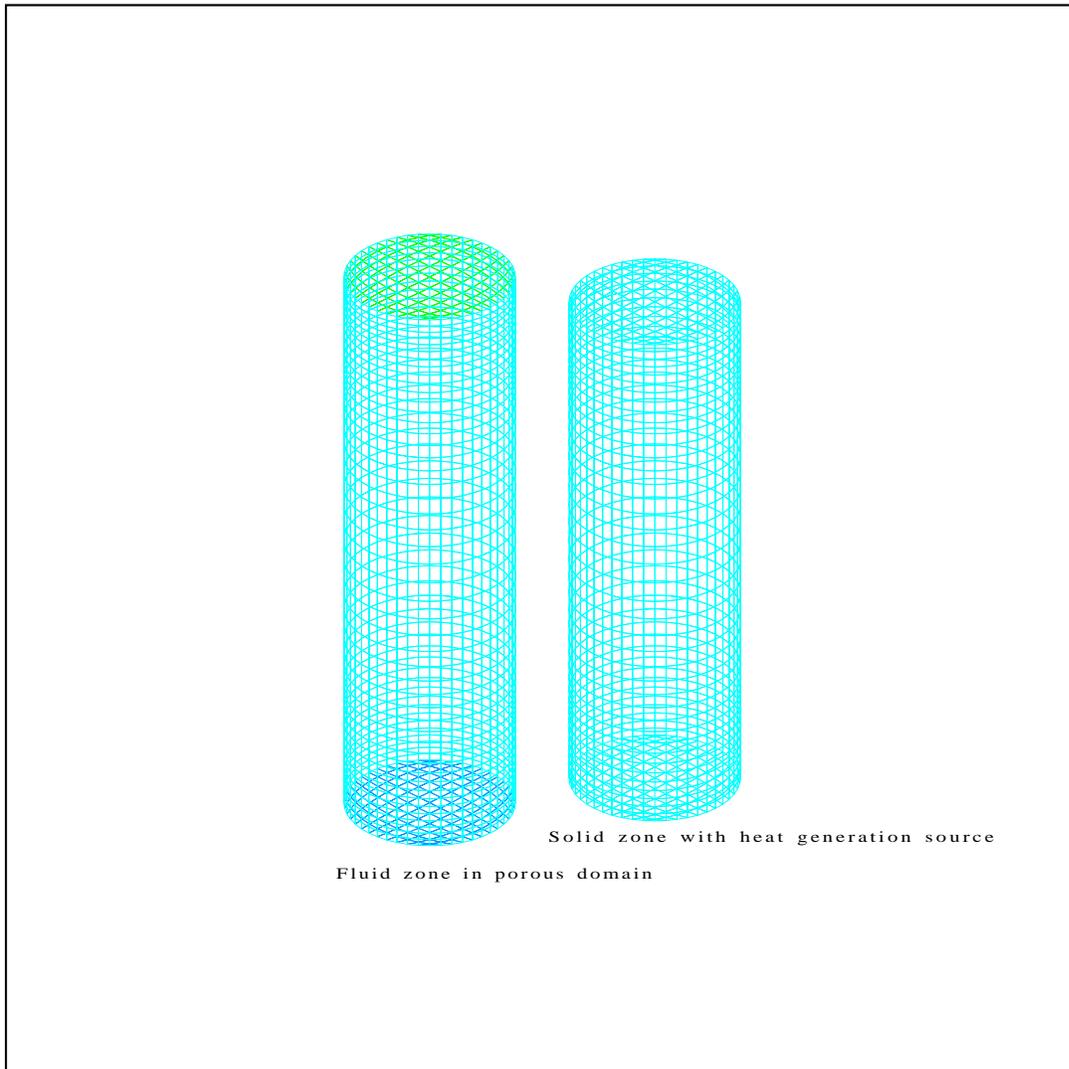OPERATIONS OF A FIXED CST BED COLUMN

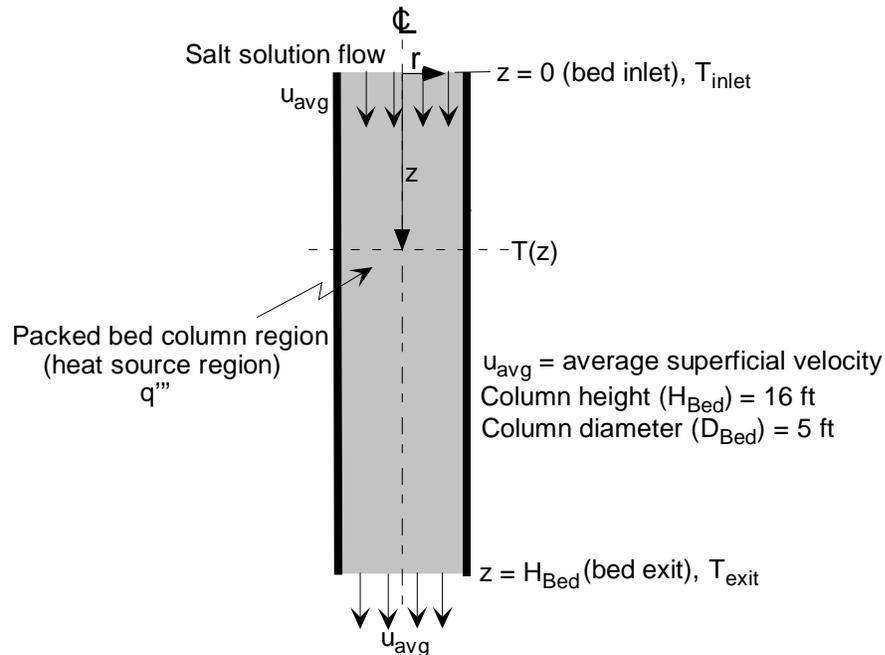Figure 7. Computational meshes for the CST heat transfer calculations

Figure 8. Theoretical approach of one-dimensional energy transport for the CST column with adiabatic wall boundary.

3. Results and Discussions

Based on the approach methodology and the modeling assumptions, theoretical and CFD analyses have been performed to compute temperature distributions within the CST modeling domain and to investigate steady-state temperature response to decay heat load of the CST column with normal process flow. This column is assumed to be cooled by natural convection or adiabatic wall boundary under the reference design conditions defined by Table 2. For natural convection boundary, heat transfer coefficient of 1.5 W/m^2K was used as discussed in the previous works [Refs. 1, 6, 9, and 15]. The thermal and material properties of the column components including the CST particle are shown in Table 4. Detailed dimensions for the CST design configurations are shown in Fig. 1 and Table 2 as modeled in the present analysis.

For the present analysis, three basic cases were theoretically considered to estimate sensitivities of temperature distributions with respect to the configurations of fluid-particle systems in a bed column. Steady-state temperature responses to uniform volumetric heat source in a fixed porous bed were estimated using the literature data. In the theoretical approach, one-dimensional approach was taken by considering overall energy balance equation for the CST column with adiabatic wall boundary condition.

The computational heat transfer approach was also taken to estimate detailed flow distribution effect on the temperature profiles for the column. In this approach, a commercial CFD code, CFX [4], was used to create prototypic geometry file under non-orthogonal mesh environment in the body-fitted coordinate system and to solve the heat transfer equations by considering conduction-convection coupled process with natural convection or adiabatic boundary conditions at the wall of the CST column. As

mentioned in the previous section, a node-mapping technique was developed to consider convection effect in the energy equation due to the fluid motion within porous media when heat source is present in solid particle region. Through the mapping algorithm, energy exchange between the solid region with heat source and the fluid region with heat sink was allowed to consider the conduction-convection coupled process in porous media. The detailed descriptions of the governing equations for the computational domain are provided in the previous report [Ref. 1]. Optimum number of meshes was obtained by the sensitivity analysis of grid fineness using the same method as the previous one. Figure 7 presents three-dimensional computational meshes for porous flow and solid zones used for the present analysis.

A theoretical approach for steady-state convection heat transfer of a fully-loaded CST column with uniform volumetric heat source was taken to compare the present computational results under the present geometrical and physical conditions as shown in Fig. 8. The results are summarized in Table 5. It is noted that there is negligible temperature difference between the center and surface of spherical particle for each of the 500 and 700 micron particles for all the cases considered here because the temperature difference is only related to the particle size and thermal property of the particle for a given heat source as shown in eq. (4a). Heat transfer for single particle surface to fluid is found to be much higher than that of a packed bed from the experimental data available in the literature as shown in Table 5.

Heat removal capability of salt solution in CST column was evaluated under 21gpm normal flow conditions. Figure 9 shows velocity vector plot of salt solution flow for uniform porous medium of the CST column with constant volumetric heat source. Temperature contour plots for the fluid and solid zones of the CST column are shown in Fig. 10. The results show that temperature near the wall boundary is higher than that of the central region of the column because of the velocity boundary layer near the no-slip wall region as shown in Fig. 11. Figure 12 presents radial temperature distributions for fluid and solid regions at the exit plane of the CST column for natural convection boundary at the column wall. These results are consistent with the theoretical results predicted by eq. (19) for constant volumetric heat source of the bed. Figure 13 illustrates qualitative results for some key operation parameters of the CST column. Average temperature difference between the solid surface and the bulk fluid region in a fixed bed is shown to be about 0.34 $^{\circ}$C as shown in Table 5. Figure 14 shows comparison of the theoretical predictions for fluid temperature with the model results along the axial flow direction. In Fig. 14, the CFD model results are based on the values averaged over the cross-sectional area of the column. The results show that about 5 $^{\circ}$C fluid temperature increases through the bed column for the present conditions shown in Table 2 and Table 4. Table 6 shows the comparison of the theoretical results with the CFD model predictions. It is noted that the CFD model prediction is about 0.2 $^{\circ}$C lower than the theoretical prediction when natural convection boundary condition is applied to the wall of the column.

The simulation results for the packed bed (Case-III) show that about 34°C maximum temperature of the CST particle was reached near the wall boundary layer of the CST column for normal operating conditions and salt solution temperature is about 1°C lower than the particle temperature for the present design and operating conditions of the CST column. In the present model, boundary condition of heat transfer at the wall of the CST column was assumed to be adiabatic or cooled by natural convection.   Table 7

summarizes maximum temperatures for process solution and CST particle for the present normal operations of a fully-loaded CST column. In this case, porosity was assumed to be uniform over the entire region of the column. In reality, the packing near the wall is usually less dense, which is closely related to the ratio of the particle diameter to the column diameter. For the present design conditions, this ratio is very large, about 3,048 for 500-micron particle, so that porosity change due to the presence of the column wall is negligible.

Table 5. Summary for the heat transfer calculation results for the three cases considered in the analysis.

Cases	Calculation Reults				
	$(T_m - T_s)_{theory}$+		Nusselt No.	Average temperature difference	
	500 microns	700 microns		$(T_s - T_f)_{theory}$**	$(T_s - T_f)_{CFD-model}$
Case-I	0.0004 ^{o}C	0.0007 ^{o}C	2.0	0.0002 ^{o}C	---
Case-II	0.0004 ^{o}C	0.0007 ^{o}C	4.51*	0.00008 ^{o}C	---
Case-III	0.0004 ^{o}C	0.0007 ^{o}C	0.001*	0.34 ^{o}C	0.34 ^{o}C

Note: * Nusselt number (Nu = $(d_p h_f)/k_f$) was evaluated by the literature correlation for
   nominal operating conditions (Re ≈ 0.23).
  ** Temperature difference was evaluated by the heat transfer correlations
     available in the literature
  + Calculated by Eq. (4a)

Table 6. Comparison of the one-dimensional theoretical predictions with the CFD model results for heat removal capability of the CST column.

Parameters	Average axial fluid temperature differences		
	Theoretical predictions*	CFD Model predictions	
		Adiabatic wall boundary	Natural convection wall boundary
$(T_{exit} - T_{inlet})_{CST-column}$	4.89 ^{o}C	4.91 ^{o}C	4.68 ^{o}C

Note: * Adiabatic boundary was assumed at the wall of the CST column based on one-
     dimensional approach.

Table 7. Comparison of maximum temperatures predicted by the CFD model of the CST column.

Items	Max. temperatures			
	Natural Convection at the Column Wall		Adiabatic Condition at the Column Wall	
	Salt solution	CST particle	Salt solution	CST particle
Inlet of the CST column	25 ^{o}C	25 ^{o}C	25 ^{o}C	25 ^{o}C
Exit of the CST column	32.3 ^{o}C	33.6 ^{o}C	32.9 ^{o}C	34.0 ^{o}C

Report: WSRC-TR-2001-00255
Date: 07/24/01

WESTINGHOUSE SAVANNAH RIVER COMPANY

HEAT TRANSFER CALCULATIONS FOR NORMAL

Page: 18 of 24

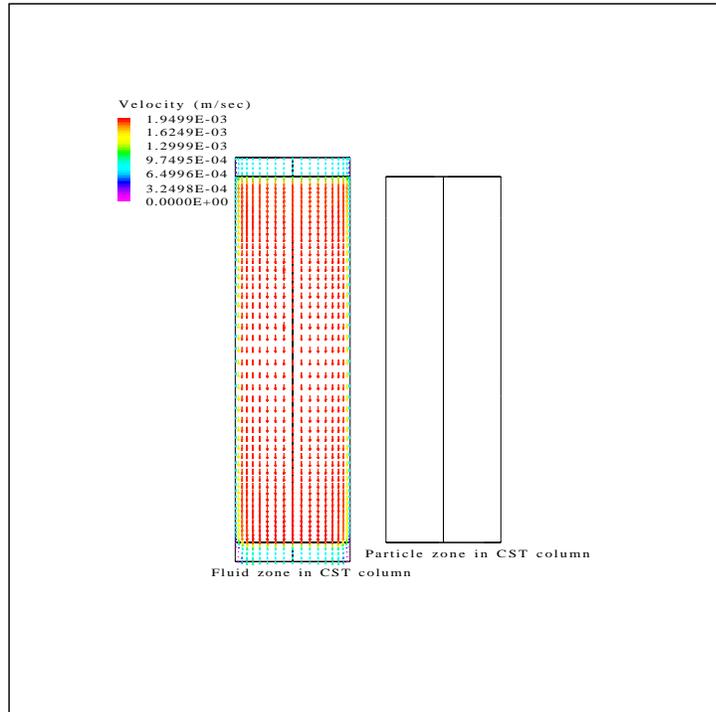OPERATIONS OF A FIXED CST BED COLUMN

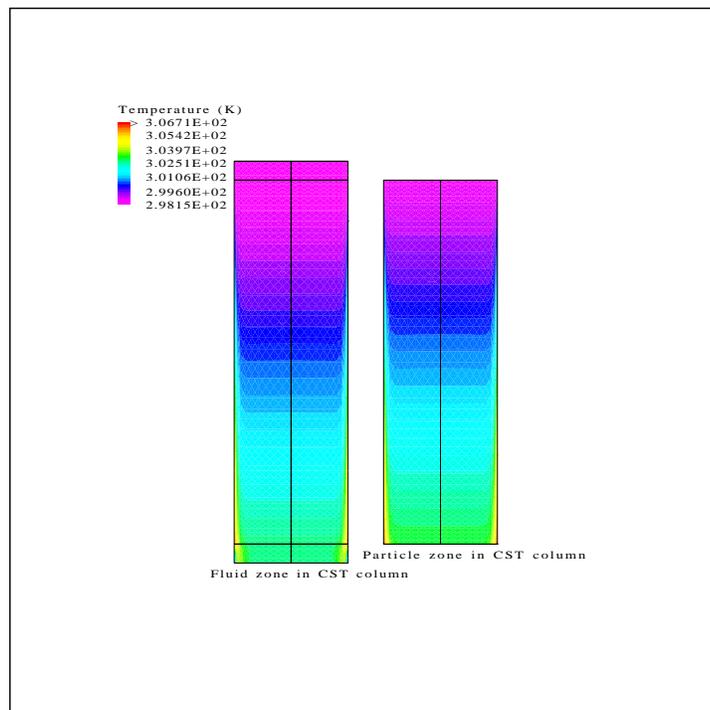Figure 9. Fluid velocity vector plot in the porous region of the CST column

Figure 10. Temperature contour plots for the fluid and solid particle zones of the CST column cooled by natural convection at the wall

WESTINGHOUSE SAVANNAH RIVER COMPANY

Report:WSRC-TR-2001-00255
Date: 07/24/01

HEAT TRANSFER CALCULATIONS FOR NORMAL
OPERATIONS OF A FIXED BED COLUMN
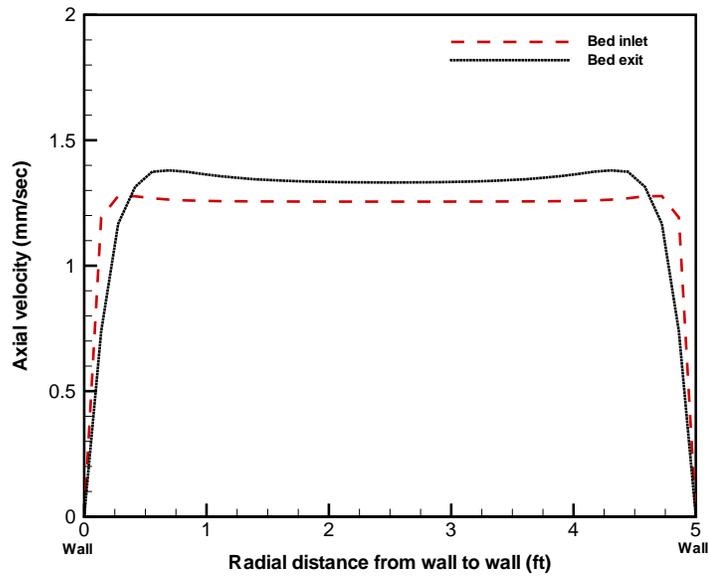
Page: 19 of 24

Figure 11. Radial interstitial velocity distributions at inlet and exit planes of the CST column
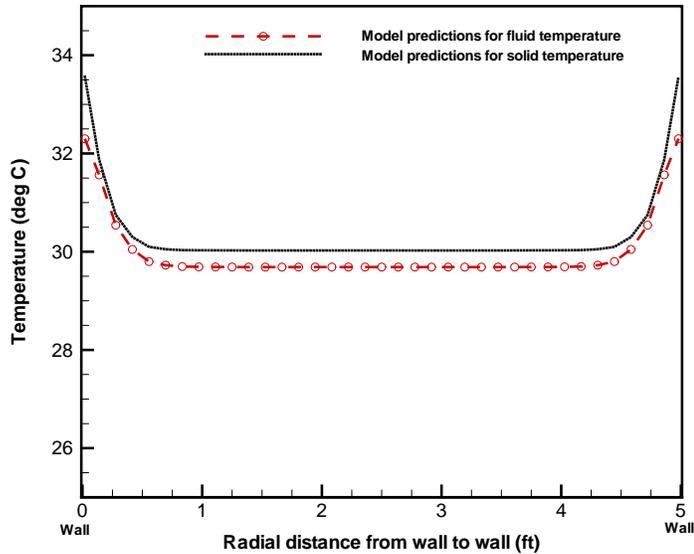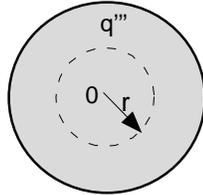

Figure 12. Comparison of radial temperature distributions for fluid and solid at the exit of the CST column for natural convection boundary conditions at the bed column wall

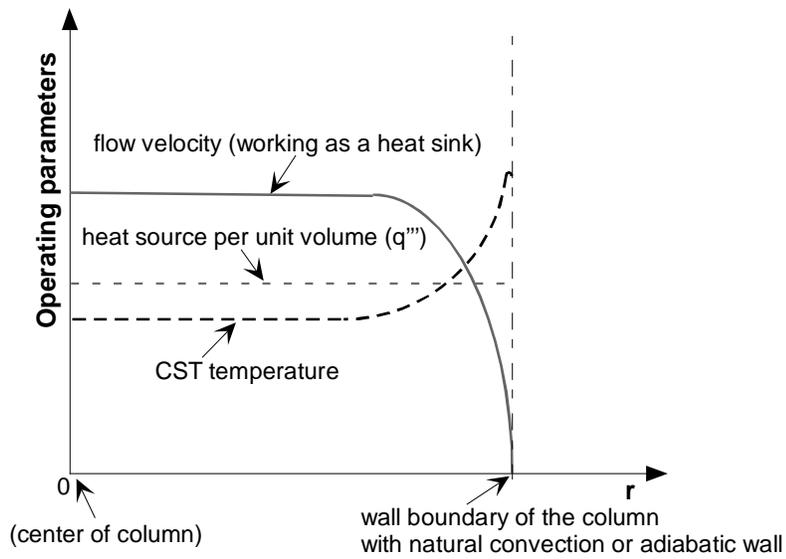(Cross-sectional area of a fully-loaded CST column)

Figure 13. Qualitative results of key operating parameters as function of radial position
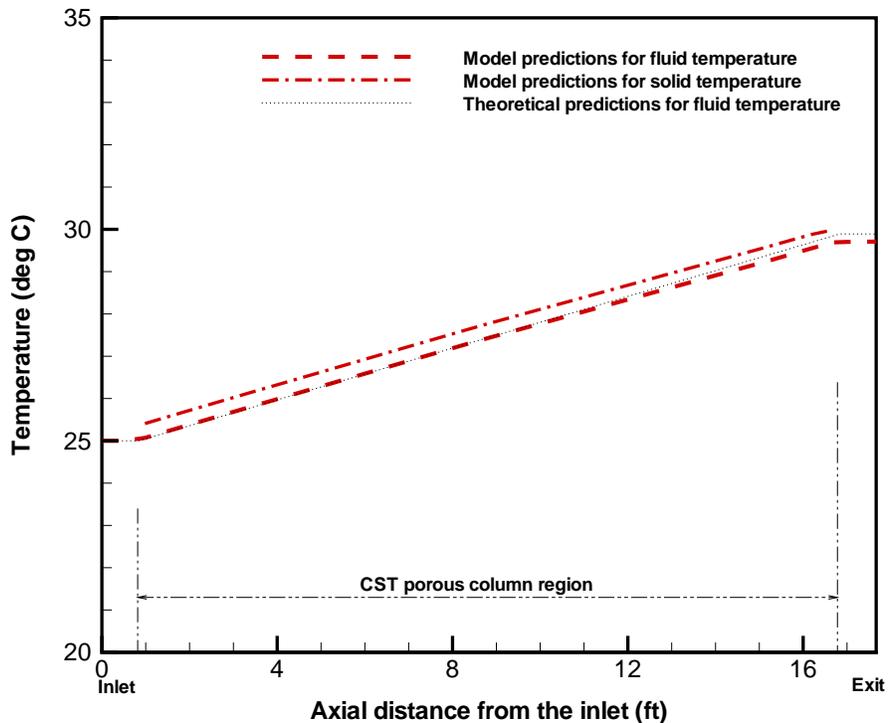at the exit of the CST column with uniform volumetric heat source

Figure 14. Comparison of axial temperature distributions along the flow direction

4. Conclusions

Heat transfer calculations for normal operating conditions of a fixed bed CST ion exchange column have been performed to assess how high the CST ion exchange system heats up during steady and downward flow operation under the reference design geometry. In the present analysis, radiation transport processes inside the CST column were assumed to be negligible compared to conduction and convection heat transfers under normal flow conditions. A boundary condition of heat transfer at the wall of the CST column was assumed to be adiabatic or cooled by natural convection.

Both theoretical and computational approaches were taken for the present work. As theoretical approach, three different configurations of fluid-particle system were considered to find the sensitivity of heat transfer capabilities with respect to operating parameters such as fluid velocity and particle packing type. For a cylindrical packed bed column under normal operating conditions (Case-III), a computational heat transfer approach was taken by using CFX, commercial computational fluid dynamics (CFD) code, to examine the multi-dimensional effect of fluid motion on the heat transfer of the column. In addition, the results computed by the present models were verified by the theoretical results. In the computational models, constant volumetric heat source for the

column was considered assuming that non-uniform local effects on the heat generation of the CST particles are negligible.

All the analysis results demonstrate that process fluid flow of the normal operating CST column provides adequate heat removal from a fully-loaded fixed bed column. Theoretical temperature distributions inside a single solid particle with uniform heat generation source indicate that the present CST particle has negligible temperature difference between the center and surface of the spherical particle containing heat source. The Case-I model investigated temperature drop across the interface of the particle-fluid for a single particle submerged in stagnant fluid system due to natural convection cooling. The Case-II model quantified temperature difference between the particle surface and its surrounding bulk fluid for the fluid-particle system with flow conditions and compared with the Case-I. The Case-III model simulated a fixed porous bed, which is close to the present CST bed column with volumetric heat source.

As expected, the results of the three models show that closely-packed bed configuration is much less coolable than dilute or loosely packed bed is. The CFD simulation results for a fully-loaded CST column show that about $34^{o}C$ maximum temperature of the CST particle was reached at the wall boundary layer of the CST column when the column has 21 gpm steady flow with $25^{o}C$ inlet temperature for normal operating conditions and the column wall is cooled by natural convection. In this case the salt solution temperature is about $1^{o}C$ lower than the particle temperature for the present operation conditions of the CST column.

From the present analysis results, main conclusions are drawn as follows:

- Under the present design and normal flow operations, the temperature difference between the CST particle and its surrounding bulk fluid is found to be less than $0.5^{o}C$.

- The coolability of the packed column containing volumetric heat source under process flow condition is much higher than the CST column with no flow.

- The impact of natural convection cooling through a fully-loaded column wall on the CST component temperatures is found to be negligible, compared to the heat removal made by forced convection during the normal operations of the present CST column system.

- From the sensitivity study of the CST column parameters, it was found that packing such as loosely or closely packed column is a key design parameter associated with the coolability of a fully-loaded CST column under flow condition since volume fraction of flowing fluid in the column, bed porosity, is closely related to the effective energy transport of the CST bed.

WESTINGHOUSE SAVANNAH RIVER COMPANY

HEAT TRANSFER CALCULATIONS FOR NORMAL
OPERATIONS OF A FIXED BED COLUMN

Report:WSRC-TR-2001-00255
Date: 07/24/01

Page: 23 of 24

5. References

1. S. Y. Lee, "Heat Transfer Calculations For a Fixed CST Bed Column", WSRC-TR-2000-00522, December 2000.

2. J. A. Pike, "Interoffice Memorandum: Input for Heat Transfer Calculations for Normal Operations of a Fixed Bed CST Ion Exchange Column", HLW-SDT-2001-00100, Rev. 0, March 20, 2001.

3. B. B. Spencer, H. Wang, K. K. Anderson, "Thermal Conductivity of IONSIVIE-911TM Crystalline Silicotitanate and Savannah River Waste Simulant Solutions", ORNL/TM-2000/285, Oah Ridge National Laboratory, TN, 2000.

4. *CFX-4.2: Environment*, AEA Technology (1997).

5. D. T. Bostick and W. V. Steele, "Thermal and Physical Property Determination for IonsivIE-911 Crystalline Silicotitanate and Savannah River Waste Simulant Solutions", WSRC-TR-99-00323, Rev. 0 (August 1999).

6. S. Y. Lee, "Three-Dimensional Thermal Analysis and Simulation of Dry Spent Nuclear Fuel Storage Canister Using CFDS-FLOW3D (U)", WSRC-TR-96-0059 (March 1996).

7. W. M. Kays and M. E. Crawford, *Convective Heat and Mass Transfer*, Second Edition, McGraw-Hill Book Company, New York (1980).

8. A. J. Chapman, *Heat Transfer*, Third Edition, Macmillan Publishing Co., Inc,, (1974).

9. C. Y. Warner and V. S. Arpaci, "An Experimental Investigation of Turbulent Natural Convection in Air at Low Pressure along a Vertical Heated Flat Plate", *International Journal of Heat and Mass Transfer*, Vol. 11, pp. 397-406 (1968).

10. Personal Communications with J. A. Pike, March 21, 2001

11. R. Rudenberg, "*The Spread of Air and Ground Fields for High Voltage Conductance Especially with Ground Connections and Short Circuits*", *Elektrotech. Z.*, Vol. 46, pp. 1342-1346 (1925).

12. H. Kramers, Physica, Vol. 12, pp. 61 (1946).

13. F. A. Zenz and D. F. Othmer, *Fluidization and Fluid-Particle Systems*, Reinhold Publishing Corp., New York, 1960.

14. D. J. Gunn and J. F. C. De Souza, "*Heat Transfer and Axial Dispersion in Packed Beds*", Chemical ngineering Science, Vol. 29, pp. 1363-1371, 1974.

15. J. Jerrell, S. Y. Lee, and A. Shadday, "Thermal Analysis of the Failed Equipment Storage Vault System (U)", WSRC-TR-95-0288 (1995).

16. R. Krupiczka, "Analysis of Thermal Conductivity in Granular Materials", International Chemical Engineering, Vol. 7, No. 1, pp. 122-144 (1967).

17. W. M. Rohsenow and H. Y. Choi, *Heat, Mass, and Momentum Transfer*, Prentice-Hall, Inc., New Jersey (1961).

18. Schack, A., *Industrial Heat Transfer*, Wiley, New York (1965).

Report: WSRC-TR-2001-00255
Date: 07/24/01

WESTINGHOUSE SAVANNAH RIVER COMPANY

HEAT TRANSFER CALCULATIONS FOR NORMAL
OPERATIONS OF A FIXED CST BED COLUMN

Page: 24 of 24

(This Page Intentionally Left Blank)