SPEEDUP (TM) Ion Exchange Column Model

by

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**T. Hang
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SpeedUp™ Ion Exchange Column Model

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SUMMARY

A transient model to describe the process of loading a solute onto the granular fixed bed in an ion exchange (IX) column has been developed using the SpeedUp™ software package. SpeedUp™ offers the advantage of smooth integration into other existing SpeedUp™ flowsheet models. The mathematical algorithm of a porous particle diffusion model was adopted to account for convection, axial dispersion, film mass transfer, and pore diffusion. The method of orthogonal collocation on finite elements was employed to solve the governing transport equations. The model allows the use of a non-linear Langmuir isotherm based on an "effective" binary ionic exchange process.

The SpeedUp™ IX column model was tested by comparing to the analytical solutions of three transport problems from the ion exchange literature. In addition, a sample calculation of a train of three crystalline silicotitanate (CST) IX columns in series was made using both the SpeedUp™ model and Purdue University's VERSE-LC code. All test cases showed excellent agreement between the SpeedUp™ model results and the test data. The model can be readily used for SuperLig™ ion exchange resins, once the experimental data are complete.

INTRODUCTION

The ion exchange technology has been considered at Department of Energy (DOE) sites to process radioactive waste. The Savannah River Site (SRS) is studying non-elutable ion exchange using CST as a potential replacement for the In-Tank Precipitation process for removing Cesium from SRS soluble radioactive waste (Beck et al., 1998). Savannah River Technology Center (SRTC) and BNFL, Inc. are conducting ion exchange tests on several elutable resins for removal of Cesium, Technetium and Sulfate from Hanford radioactive waste (WFO-98-003). Computer models have been developed independently by Professor R.G. Anthony (Department of Chemical Engineering, Texas A&M University) and Professor N.-H. Wang (School of Engineering, Purdue University) to calculate IX column size and performance to provide a basis for preliminary design of SRS salt decontamination process (Walker, 1998). A PC-based version of Professor Wang's VERSE-LC (Versatile Reaction Separation simulator for Liquid Chromatography) software to model liquid adsorption, ion exchange and liquid chromatography processes (Whitley and Wang, 1998) has been licensed to SRTC to assist in the lab-scale column tests for both the SRS and BNFL programs. VERSE-LC has been thoroughly verified by SRTC researchers (Hamm et al., 1999). It is of great interest to develop a sophisticated IX column model as an integral part of the existing SRS and BNFL SpeedUp™

flowsheet models. Additionally, the SpeedUp™ modeling structure allows the model to be easily modified and expanded to account for chemical changes, temperature effect, elution of resins etc. in the future revisions. This report summarizes the SpeedUp™ IX column model development and verification.

MODEL DEVELOPMENT

Assumptions

The SpeedUp™ model for IX column describes the ion exchange loading of a solute onto the granular resin fixed bed as an adsorption process. The mathematical method applicable to mass transfer in a porous medium is utilized to account for bulk convection, axial dispersion, film mass transfer, pore diffusion, and adsorption. For simplicity, the method involves the following basic assumptions:

1. The solution contains only two components, i.e. a solvent and a single solute.
2. Plug flow with constant volumetric flow rate through the packed column.
3. No radial concentration gradients in the column.
4. Isothermal process within the column.
5. Solid particles are spherical, uniform in size, and do not swell or shrink.
6. Negligible surface diffusion with Fickian pore diffusion dominating.
7. No angular concentration gradients within a particle.
8. Constant pore diffusivity.
9. Local equilibrium between the solute concentration adsorbed on the solid and the local solute concentration in the solution.

Governing Equations

A porous particle diffusion model proposed for simulation of fixed-bed adsorption processes (Berninger et al., 1991) was adopted for the SpeedUp™ IX column model. The porous particle diffusion model provides the material balance equations in both the mobile phase and the pore phase. An "effective" binary solute-solvent system is assumed. Furthermore, for ionic species modeling, the total ionic strength of the feed solution is assumed to be equal to the native solution within the column. This assumption is not typically limiting for the ion exchange systems of general interest for DOE applications.

Mobile phase:

$$\frac{\partial C}{\partial t} = E_b \frac{\partial^2 C}{\partial z^2} - u_o \frac{\partial C}{\partial z} - \frac{3k_f(1-\epsilon_b)}{R_p \epsilon_b} (C - C_{p,r=R_p}) \quad (1)$$

$$z = 0: \quad E_b \frac{\partial C}{\partial z} = u_o (C(t,0) - C_o) \quad (2)$$

$$z = L: \quad \frac{\partial C}{\partial z} = 0 \quad (3)$$

$$t = 0: \quad C = C(0, z) \quad (4)$$

Pore phase:

$$\left(\varepsilon_p + (1 - \varepsilon_p) \frac{\partial Q}{\partial C_p} \right) \frac{\partial C_p}{\partial t} = \varepsilon_p \frac{D_p}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial C_p}{\partial r} \right) \quad (5)$$

$$r = 0: \quad \frac{\partial C_p}{\partial r} = 0 \quad (6)$$

$$r = R_p: \quad \varepsilon_p D_p \frac{\partial C_p}{\partial r} = k_f (C - C_{p,r=R_p}) \quad (7)$$

$$t = 0: \quad C_p = C_p(0, r) \quad (8)$$

The axial dispersion coefficient, E_b , is estimated by the Chung and Wen correlation (Chung and Wen, 1968):

$$\frac{u_o L}{E_b} = \frac{L}{2\varepsilon_b R_p} (0.2 + 0.011 \text{Re}^{0.48}) \quad (9)$$

The Reynolds number, Re , in Equation 9 is defined as:

$$\text{Re} = \frac{2R_p \rho u_o \varepsilon_b}{\mu} \quad (10)$$

The Wilson and Geankoplis (Wilson and Geankoplis, 1966) correlation is used to determine the film mass transfer coefficient, k_f :

$$\left(\frac{k_f}{u_o \varepsilon_b} \right) \text{Sc}^{2/3} = \frac{1.09}{\varepsilon_b} \text{Re}^{-2/3} \quad (11)$$

With the Schmidt number, Sc , defined as:

$$\text{Sc} = \left(\frac{\mu}{\rho D_\infty} \right) \quad (12)$$

For our applications, the "effective" intraparticle diffusivity, D_p , is fitted to column experimental data.

Solid phase concentrations Q are related to pore phase concentrations C_p by isotherms. The non-

linear Langmuir isotherm is selected to represent the Q-C_p relationship:

$$Q = \frac{aC_p}{1 + bC_p} \quad (13)$$

Numerical Method

The method of orthogonal collocation on finite elements is applied to numerically solve Equations (1) and (5). The method provides a mathematical technique in which a series of orthogonal polynomials are used as trial functions, the collocation points are taken as the roots to one of those polynomials, and the dependent variables are the solution values at the collocation points. The entire domain is divided into a set of elements. Orthogonal polynomials defined for each element are pieced together to provide an approximation over the whole domain (Finlayson, 1980). The first and second spatial derivatives at any interior collocation point can be expressed in matrix notation:

$$\frac{\partial u_h}{\partial x} = \sum_{k=1}^{N+2} A_{hk} u_k \quad (14)$$

$$\frac{1}{x^{m-1}} \frac{\partial}{\partial x} \left[x^{m-1} \frac{\partial u_h}{\partial x} \right] = \sum_{k=1}^{N+2} B_{hk} u_k \quad (15)$$

where $m = 1, 2$, or 3 for planar, cylindrical and spherical geometry, respectively. Non-symmetric polynomials are used in the axial direction (planar), and symmetric polynomials are used in the spherical (pore phase) direction. Appendix A lists the values of matrices A and B for the symmetric and non-symmetric polynomials at a specified number of interior collocation points.

At each elemental node, boundary conditions must be specified. At interior elemental nodes, the boundary conditions are those of continuity. At exterior nodes, boundary equations (2) and (3) for the mobile phase or (6) and (7) for the pore phase are used (Berninger et al., 1991). Applying the orthogonal collocation technique, the second-order partial differential equations and their associated boundary conditions representing the pore diffusion model can be converted into a set of ordinary differential and algebraic equations.

Mobile phase:

$$\frac{\partial C_h}{\partial t} = \frac{D_b}{\Delta z^2} \sum_{k=1}^{N_a+2} B_{hk} C_k - \frac{u_o}{\Delta z} \sum_{k=1}^{N_a+2} A_{hk} C_k - \frac{3k_f(1-\varepsilon_b)}{R_p \varepsilon_b} (C_h - C_{p,h(N_p+1)}) \quad (16)$$

$$z = 0: \quad D_b \sum_{k=1}^{N_a+2} A_{1k} C_k = u_o (C_1 - C_o) \quad (17)$$

$$z = L: \quad \sum_{k=1}^{N_a+1} A_{(N_a+2)k} C_k = 0 \quad (18)$$

$$t = 0: \quad C_h = C_h(t = 0) \quad (19)$$

Pore phase:

$$\left(\varepsilon_p + (1 - \varepsilon_p) \frac{\partial q_{hl}}{\partial C_{p,hl}} \right) \frac{\partial C_{p,hl}}{\partial t} = \frac{\varepsilon_p D_p}{R_p^2} \sum_{k=1}^{N_p+1} B_{S,lk} C_{p,hk} \quad (20)$$

$$r = R_p: \quad \varepsilon_p D_p \sum_{k=1}^{N_p+1} A_{S,lk} C_{p,k} = k_f (C_h - C_{p,h(N_p+1)}) \quad (21)$$

$$t = 0: \quad C_{p,hl} = C_{p,hl}(t = 0) \quad (22)$$

Index h is for interior collocation point in the axial direction. Index l is for interior collocation point in the radial direction (pore phase). The boundary condition at $r = 0$ is not needed because it is already built into the symmetric polynomial. For clarification, Figure 1 below illustrates the grid arrangement in the orthogonal collocation method.

Figure 1: Orthogonal Collocation on Finite Elements – Computational Grid

(Example shown: 3 interior collocation points per axial element,
4 interior collocation points in the particle element)

SpeedUp™ Modeling

The IX column model was created using the SpeedUp™ software package marketed by Aspen Technology (Aspen Technology, 1993). SpeedUp™ provides the architecture, upon which models are built, as well as the algorithms to solve the model equations. The SpeedUp™ equation solvers are exceptionally robust and very well suited to solving a system of differential and algebraic equations. Complex dynamic models have been successfully developed by researchers at SRS (Aull et al., 1994; Gregory et al., 1994; Hang et al., 1994; Smith, 1995). A SpeedUp™ IX column model also offers the advantages of smooth integration into the existing SpeedUp™ flowsheet models and easy modifications to expand capabilities.

MODEL VERIFICATION

The SpeedUp™ IX column model was tested by comparing to several transport problems from the ion exchange literature presented in the VERSE-LC verification work (Hamm, 1999). The model calculated results were compared to analytical solutions. In addition, a sample calculation of an IX train consisting of three CST IX columns in series was made using both the SpeedUp™ IX column model and the VERSE-LC code. SpeedUp™ calculations were performed on the IBM RS/6000 workstation. The VERSE-LC code was executed on the IBM Intel™ Pentium II/400Mhz Personal Computer running Microsoft Windows 95.

The following test cases were used to verify the SpeedUp™ IX column model:

- Analytical Test Case 1: Unretarded transport of a single species with low hydrodynamic dispersion.
- Analytical Test Case 2: Unretarded transport of a single species with a higher degree of hydrodynamic dispersion.
- Analytical Test Case 3: Retarded transport of a single species with a higher degree of hydrodynamic dispersion.
- Three-Column Carousel Test Case: This test case involves the calculation of a train of three CST IX columns in series. A fourth column loaded with fresh resin is in standby to be used when the first column is loaded and rotated out of service at the end of a cycle. Cycle time, total Cesium loading, and the column change-over operation in each cycle are to be simulated.

The parameters employed in the SpeedUp™ IX column model are summarized in Table 1. In the current SpeedUp™ IX model, three interior collocation points per axial element and four interior collocation points in the particle element are specified. This discretization scheme seems adequate for most systems. The number of axial elements can be varied to achieve the desired accuracy. The effects of these parameters (i.e. number of axial elements N_z , number of interior axial collocation points N_a , and number of interior particle collocation points N_p) on the convergence of the system and the computational speed have been studied elsewhere (Berninger et al., 1991).

Table 1: SpeedUp™ Model Parameter Settings

Parameters	Analytical Test Case 1	Analytical Test Case 2	Analytical Test Case 3	3-Column Carousel Test Case
Column length L	500 cm	500 cm	500 cm	16 ft/column
Column diameter d	10 cm	10 cm	10 cm	5 ft
Particle radius R_p	200 μm	200 μm	100 μm	187.5 μm
Bed porosity ε_b	0.3	0.3	0.3	0.5
Particle porosity ε_p	0.001	0.001	0.001	0.24
Interstitial velocity u_o	6.6667 cm/min	6.6667 cm/min	6.6667 cm/min	8.7563 cm/min
Bulk bed density ρ_b	0.7 g/ml	0.7 g/ml	0.7 g/ml	1.0 g/ml
Solid density ρ_s	1.0 g/ml	1.0 g/ml	1.0 g/ml	2.6316 g/ml
Inlet solution concentration	1.0 mg/ml	1.0 mg/ml	1.0 mg/ml	0.0182 mg/ml
Axial dispersion coefficient E_b	6.667 cm^2/min	20 cm^2/min	20 cm^2/min	0.796 cm^2/min
Intraparticle diffusivity D_p	5E-5 cm^2/min	5E-5 cm^2/min	1E-1 cm^2/min	5E-5 cm^2/min
Film mass transfer coefficient k_f	0.0 cm/min	0.0 cm/min	3 cm/min	0.2374 cm/min
Langmuir coefficient a	0.0 mg/ml	0.0 mg/ml	0.3 mg/ml	2562 mg/ml
Langmuir coefficient b	0.0 ml/mg	0.0 ml/mg	0.0 ml/mg	33.26 ml/mg
Number of axial elements N_z	50	50	50	50/column
Number of interior axial collocation points N_a	3	3	3	3
Number of interior particle collocation points N_p	4	4	4	4
Time duration	50 min	50 min	50 min	Cycle time (determined by Cesium concentration reaching 1.3E-6 mg/ml at the exit of the second column)

Analytical Test Case 1

The three analytical test cases selected deal with the problem of a one-dimensional (1-D) advection-dispersion of a non-conservative solute species through a semi-infinite porous medium for groundwater modeling. For ion exchange modeling, the problem can be reformulated as a packed bed of stationary nonporous particles. The 1-D advection-dispersion equation facilitates testing an algorithm's behavior over a wide range of conditions. In the analytical test case 1, the problem of unretarded transport of a single species with low hydrodynamic dispersion was considered. Figure 2 provides a comparison of the SpeedUp™ model results to the analytical data. Two hundred finite elements, each with 3 interior collocation points, were employed in the SpeedUp™ simulation. Excellent agreement was achieved as shown in Figure 2.

Figure 2: Relative Solute Concentration Profile Comparison for Analytical Test Case 1

Analytical Test Case 2

In this case, the problem of unretarded transport of a single species with a higher degree of hydrodynamic dispersion was studied. The longitudinal (axial) dispersion coefficient was increased by a factor of 3 over the value used in the analytical test case 1. With increasing axial dispersion the concentration profiles are expected to be less steep. Figure 3 displays a comparison of the SpeedUp™ model results to the analytical data for concentration profiles at 25 and 50 minutes. Again, excellent agreement was achieved.

Figure 3: Relative Solute Concentration Profile Comparison for Analytical Test Case 2

Analytical Test Case 3

This case was to deal with retarded transport of a single species with a higher degree of hydrodynamic dispersion. The problem of particle adsorption was simulated in the SpeedUp™ model by selecting a high film mass transfer coefficient, k_f (e.g. 3 cm/min), to achieve local adsorption equilibrium at the particle surfaces. In addition, a large pore diffusivity, D_p (e.g. 0.1 cm²/min), was used to minimize any concentration profile gradients within the pores. A linear isotherm corresponding to the solute distribution coefficient k_d of the analytical test case was obtained by setting the second Langmuir parameter, b , to zero. Note that as a result of retardation the concentration profiles in the C/C_0 vs. z/L plot are shifted back and become steeper. Figure 4 shows an excellent comparison of the SpeedUp™ results to the analytical data.

Figure 4: Relative Solute Concentration Profile Comparison for Analytical Test Case 3

Three-Column Carousel Test Case

This case was designed to test the ability of the SpeedUp™ model to computing an actual design case of the CST IX columns for removing Cesium from SRS soluble radioactive waste. The carousel arrangement is made up of three columns in series with a fourth column loaded with fresh resin in standby. At the time when Cesium concentration at the exit of the second column reaches 1.3×10^{-6} mg/ml, the first column is taken out of service, the second column becomes the lead column, the third column becomes the middle column and the fresh, standby column becomes the third or guard column at the end of the train. The results from the SpeedUp™ simulations are compared to those obtained from the VERSE-LC code for the same problem. Since VERSE-LC has been extensively verified (Hamm et al., 1999), the comparison will indicate how adequate and optimal the numerical solutions performed by the SpeedUp™ model are. The entire SpeedUp™ model set up for the three-column carousel test case is discussed at length in Appendix B. Table 2 below provides the sample of the VERSE-LC input file for this test case.

Table 2: VERSE-LC Input File for the Three-Column Carousel Test Case

Simulation of large scale removal of Cs (16ft long x 5ft diameter)	
SRS avg waste; 3-column carousel; 21.16 gpm	
1, 750, 6, 4	ncomp, nelem, ncol-bed, ncol-part
MCWNA	isotherm, axial-disp, film-coef, surf-diff, BC-col
NNN	input-only, perfusable, feed-equil, datafile.yio
G	comp-conc units
1463.0, 152.4, 79863.5, 0.0d0	Length(cm), Diam(cm), Q-flow(ml/min), CSTR vol(ml)
187.5, 0.5, 0.24, 0.0	part-rad(μ m), bed-void, part-void, sorb-cap()
0.0	init-conc(mg/ml)
S	COMMAND - conc step change
1, 0.0, 0.0182073, 1, 0.0	spec id, time(min), conc(mg/ml), freq, dt(min)
m	COMMAND - Carousel-Conc. Driven
250, 500, 0, 1, 1.3d-6, 0.0, 1500000	
D	COMMAND - dump column profile
-1, 72000, 1, 0.0	part pt (-1 all), time(min), freq, dt(min)
D	COMMAND - dump column profile
-1, 144000, 1, 0.0	part pt (-1 all), time(min), freq, dt(min)
D	COMMAND - dump column profile
-1, 216000, 1, 0.0	part pt (-1 all), time(min), freq, dt(min)
D	COMMAND - dump column profile
-1, 288000, 1, 0.0	part pt (-1 all), time(min), freq, dt(min)
D	COMMAND - dump column profile
-1, 360000, 1, 0.0	part pt (-1 all), time(min), freq, dt(min)
h	COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1	unit op#, ptscale(1-4) filtering
h	COMMAND - effluent history dump
3, 1.0, 1.0, 0.25, 0.1	unit op#, ptscale(1-4) filtering
h	COMMAND - effluent history dump
4, 1.0, 1.0, 0.25, 0.1	unit op#, ptscale(1-4) filtering
-	end of commands
1500000, 10.0	end time(min), max dt in B.V.s
1.0d-7, 1.0d-4	abs-tol(mg/ml), rel-tol
-	non-negative conc constraint
1.0d0	size exclusion factor
5.00d-5	part-pore diffusivities(cm^2/min)
6.44d-4	Brownian diffusivities(cm^2/min)
2562	Multi-Langmuir a (ml/ml B.V.)
33.26	Multi-Langmuir b (ml/mg)

Figure 5 shows the comparison for relative Cesium concentration profile in the first column requested at 1200 hours and 2400 hrs of the first cycle. The results predicted by both models were almost identical. In Figure 6, Cesium concentration at the exit of the first column was calculated for over eight cycles. As Figure 6 indicates, very good agreement was again achieved.

Figure 5: Relative Cesium Concentration Profile Comparison for Column 1/Cycle 1 Three-Column Carousel Test Case

Figure 6: Cesium Concentration at Column 1 Exit for Three-Column Carousel Test Case

CONCLUSIONS

A computer model for non-elutable ion exchange was developed using Aspen Technology's SpeedUp™ software package. The SpeedUp™ IX column model provides smooth integration to the existing SpeedUp™ flowsheet models. For verification, the model calculated results were compared to the solutions of three analytical test cases. Additionally, a complex column switching operation of a three-column IX carousel was simulated by both the SpeedUp™ IX column model and Purdue University's VERSE-LC code. All test cases show excellent agreement between the SpeedUp™ model results and the test data.

NOMENCLATURE

a	Langmuir coefficient, mg/ml B.V. (B.V.: Volume of the fixed bed)
A_{hk}	First derivative matrix involving non-symmetric polynomials
$A_{S,hk}$	First derivative matrix involving symmetric polynomials
b	Langmuir coefficient, ml/mg
B_{hk}	Second derivative matrix involving non-symmetric polynomials
$B_{S,hk}$	Second derivative matrix involving symmetric polynomials
C	Bulk-phase solute concentration, mg/ml
C_p	Pore-phase solute concentration, mg/ml
C_o	Column inlet solute concentration, mg/ml
D_{∞}	Brownian diffusivity, cm^2/min
E_b	Axial dispersion coefficient, cm^2/min
k_f	Film mass transfer coefficient, cm/min
L	Column length, cm
N_a	Number of interior axial collocation points
N_p	Number of interior particle collocation points
N_z	Number of axial elements
Q	Solid-phase solute concentration, mg/ml S.V. (S.V.: Volume of the solid phase)
r	Radial position from center of adsorbent particle, cm
Re	Reynolds number
R_p	Adsorbent particle radius, cm
Sc	Schmidt number
T	Time, min
u_o	Linear interstitial velocity, cm/min
z	Position in axial direction, cm
ϵ_b	Bed porosity
ϵ_p	Intraparticle porosity
μ	Viscosity, $\text{g s}^{-1} \text{cm}^{-1}$
ρ	Density, g/ml
ρ_b	Bulk bed density, g/ml
ρ_s	Solid density, g/ml

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APPENDIX A MATRICES FOR ORTHOGONAL COLLOCATION

In the orthogonal collocation method, the first and second derivatives are evaluated at the collocation points as in the following matrix form (Finlayson, 1980):

$$\frac{dy}{dx} = Ay$$

$$\nabla^2 y \equiv \frac{1}{x^{m-1}} \frac{d}{dx} \left(x^{m-1} \frac{dy}{dx} \right) = By$$

where $m = 1, 2$, or 3 for planar, cylindrical, or spherical geometry, respectively. Values of matrices A and B for non-symmetric and symmetric polynomials are provided below.

Matrices for Orthogonal Collocation for Non-Symmetric Polynomials (Planar Geometry)

One Interior Collocation Point

INTERIOR COLLOCATION PTS POINT	ORDINATE
-----------------------------------	----------

1	0.50000000
---	------------

A:

-3.00000	4.00000	-1.00000
-1.00000	0.00000	1.00000
1.00000	-4.00000	3.00000
0.00000	0.00000	0.00000
0.00000	0.00000	0.00000
0.00000	0.00000	0.00000
0.00000	0.00000	0.00000
0.00000	0.00000	0.00000
0.00000	0.00000	0.00000

B:

4.00000	-8.00000	4.00000
4.00000	-8.00000	4.00000
4.00000	-8.00000	4.00000
0.00000	0.00000	0.00000
0.00000	0.00000	0.00000
0.00000	0.00000	0.00000
0.00000	0.00000	0.00000
0.00000	0.00000	0.00000
0.00000	0.00000	0.00000

Two Interior Collocation Points

INTERIOR COLLOCATION PTS POINT	ORDINATE
-----------------------------------	----------

1	0.21132487
2	0.78867513

A:

-7.00000	8.19615	-2.19615	1.00000
-2.73205	1.73205	1.73205	-0.73205

0.73205	-1.73205	-1.73205	2.73205
-1.00000	2.19615	-8.19615	7.00000
0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000

B:

24.00000	-37.17691	25.17692	-12.00000
16.39231	-24.00000	12.00000	-4.39231
-4.39230	12.00000	-24.00000	16.39230
-12.00000	25.17691	-37.17691	24.00000
0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000

Three Interior Collocation Points

INTERIOR COLLOCATION PTS	
POINT	ORDINATE
1	0.11270165
2	0.50000000
3	0.88729835

A:

-13.00000	14.78830	-2.66667	1.87836	-1.00000
-5.32379	3.87298	2.06559	-1.29099	0.67621
1.50000	-3.22749	0.00000	3.22749	-1.50000
-0.67621	1.29099	-2.06559	-3.87298	5.32379
1.00000	-1.87836	2.66667	-14.78831	13.00000
0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000

B:

84.00001	-122.06316	58.66666	-44.60350	24.00000
53.23790	-73.33334	26.66667	-13.33334	6.76210
-6.00000	16.66667	-21.33333	16.66667	-6.00000
6.76210	-13.33333	26.66666	-73.33334	53.23790
24.00000	-44.60350	58.66666	-122.06319	84.00001
0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000

Four Interior Collocation Points

INTERIOR COLLOCATION PTS	
POINT	ORDINATE
1	0.06943184
2	0.33000946
3	0.66999054
4	0.93056816

A:

-21.00000	23.63045	-3.67988	1.81255	-1.76312	1.00000
-8.77831	6.66400	2.84048	-1.23246	1.16126	-0.65497

2.49525	-5.18482	0.76883	2.94134	-2.24965	1.22906
-1.22906	2.24965	-2.94134	-0.76883	5.18482	-2.49525
0.65497	-1.16126	1.23246	-2.84048	-6.66400	8.77831
-1.00000	1.76312	-1.81255	3.67988	-23.63045	21.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

B:

220.00000	-311.79837	132.25317	-70.71658	70.26179	-40.00000
135.86383	-183.02968	59.65936	-20.53064	18.17426	-10.13711
-11.28545	31.82235	-36.97033	21.82574	-10.95107	5.55875
5.55874	-10.95107	21.82574	-36.97033	31.82235	-11.28545
-10.13711	18.17426	-20.53064	59.65935	-183.02969	135.86383
-40.00000	70.26178	-70.71658	132.25316	-311.79837	220.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Five Interior Collocation Points

INTERIOR COLLOCATION PTS

POINT	ORDINATE
-------	----------

1	0.04691008
2	0.23076534
3	0.50000000
4	0.76923466
5	0.95308995

A:

-31.00000	34.69972	-5.03152	2.13333	-1.50942	1.70788	-1.00000
-13.09609	10.13408	3.87973	-1.44628	0.98752	-1.10353	0.64458
3.73216	-7.62512	1.51671	3.41215	-1.85712	1.94084	-1.11962
-1.87500	3.36805	-4.04306	0.00000	4.04306	-3.36806	1.87500
1.11962	-1.94084	1.85712	-3.41215	-1.51671	7.62512	-3.73216
-0.64458	1.10353	-0.98752	1.44628	-3.87973	-10.13410	13.09610
1.00000	-1.70788	1.50942	-2.13333	5.03151	-34.69973	31.00001
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

B:

480.00000	-671.96838	268.34686	-123.73331	89.65969	-102.30492	60.00003
292.91504	-390.42096	120.83913	-35.69749	22.74945	-24.80218	14.41698
-21.02473	59.81682	-66.91239	35.69749	-12.53116	11.26126	-6.30729
7.50000	-14.86705	30.03371	-45.33333	30.03371	-14.86705	7.50001
-6.30728	11.26125	-12.53116	35.69749	-66.91238	59.81683	-21.02475
14.41698	-24.80219	22.74947	-35.69752	120.83916	-390.42120	292.91528
59.99999	-102.30488	89.65968	-123.73330	268.34683	-671.96863	480.00024
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Six Interior Collocation Points

INTERIOR COLLOCATION PTS

POINT	ORDINATE
-------	----------

1	0.03376526
2	0.16939530
3	0.38069040
4	0.61930960

5 0.83060467

6 0.96623474

A:

-42.99999	47.98975	-6.68415	2.61671	-1.60850	1.36318	-1.67701	1.00000
-18.27727	14.29064	5.15197	-1.77204	1.04990	-0.87692	1.07242	-0.63870
5.21376	-10.55152	2.34971	4.16381	-1.95547	1.51238	-1.79597	1.06331
-2.63694	4.68872	-5.37935	0.50605	4.19078	-2.52633	2.77799	-1.62093
1.62093	-2.77799	2.52633	-4.19078	-0.50605	5.37935	-4.68872	2.63694
-1.06331	1.79598	-1.51238	1.95547	-4.16382	-2.34970	10.55152	-5.21376
0.63870	-1.07242	0.87692	-1.04990	1.77204	-5.15197	-14.29064	18.27727
-1.00000	1.67701	-1.36318	1.60850	-2.61672	6.68415	-47.98976	42.99999

B:

923.99976	-1284.56531	495.91891	-211.29018	133.13629	-113.95101	140.75165	-83.99995
560.22040	-742.28186	223.22067	-60.86293	33.59371	-27.26437	32.95134	-19.57698
-37.05573	106.00676	-116.34000	58.97980	-17.88219	11.68188	-12.94777	7.55723
11.18459	-22.28468	45.47341	-65.37791	39.36675	-13.78716	12.30019	-6.87518
-6.87519	12.30019	-13.78717	39.36675	-65.37791	45.47340	-22.28467	11.18458
7.55722	-12.94776	11.68188	-17.88218	58.97979	-116.33997	106.00679	-37.05574
-19.57699	32.95135	-27.26438	33.59371	-60.86294	223.22061	-742.28174	560.22021
-84.00000	140.75169	-113.95107	133.13631	-211.29025	495.91882	-1284.56555	923.99969

Matrices for Orthogonal Collocation for Symmetric Polynomials (Spherical Geometry)

One Interior Collocation Point

THE COLLOCATION POINTS ARE

0.77460E+00 0.10000E+01

A:

-3.87298	3.87298
-5.00000	5.00000

B:

-15.00000	15.00000
-15.00000	15.00000

Two Interior Collocation Points

THE COLLOCATION POINTS ARE

0.53847E+00 0.90618E+00 0.10000E+01

A:

-3.54403	8.04919	-4.50516
-0.85930	-6.72235	7.58165
0.94827	-14.94828	14.00001

B:

-13.59531	20.42831	-6.83301
14.57171	-91.40476	76.83305
24.05442	-129.05447	105.00006

Three Interior Collocation Points

THE COLLOCATION POINTS ARE

0.40585E+00 0.74153E+00 0.94911E+00 0.10000E+01

A:

-4.18187	8.20265	-10.19101	6.17023
-0.98927	-3.67021	10.03434	-5.37484
0.27903	-2.27801	-11.14859	13.14760
-0.37710	2.72364	-29.34654	27.00003

B:

-20.02574	26.60195	-12.57212	5.99591
10.87790	-44.91904	51.74983	-17.70865
-6.77880	68.23693	-313.05557	251.59755
-19.68847	131.04352	-489.35522	378.00031

Four Interior Collocation Points

THE COLLOCATION POINTS ARE

0.32425E+00 0.61337E+00 0.83603E+00 0.96816E+00 0.10000E+01

A:

-4.98836	9.36546	-9.51916	13.39168	-8.24962
-1.15593	-3.42882	8.46320	-9.59689	5.71845
0.32306	-2.32708	-4.57116	13.82877	-7.25359
-0.13542	0.78621	-4.11991	-16.99869	20.46787
0.19631	-1.10257	5.08667	-48.18018	43.99976

B:

-29.31681	38.02225	-13.89345	11.16665	-5.97860
12.73519	-48.58884	47.69691	-23.08930	11.24609
-3.61367	37.03847	-110.32513	117.18764	-40.28716
4.81349	-29.71621	194.22569	-801.76575	632.44220
16.98878	-93.27109	395.30963	-1309.02344	989.99658

Five Interior Collocation Points

THE COLLOCATION POINTS ARE

0.26954E+00 0.51910E+00 0.73015E+00 0.88706E+00 0.97823E+00 0.10000E+01

A:

-5.85556	10.78172	-10.19315	11.78708	-17.14737	10.62733
-1.34021	-3.60005	8.70972	-7.96043	10.79117	-6.60023
0.36427	-2.50402	-3.61805	10.32157	-11.13108	6.56718
-0.15912	0.86438	-3.89824	-5.85287	18.79050	-9.74478
0.07868	-0.39837	1.42910	-6.38772	-24.24637	29.52452
-0.11784	0.58900	-2.03961	8.01569	-71.44629	64.99890

B:

-41.03722	52.79892	-17.94175	10.94133	-10.93856	6.17755
16.04351	-59.50291	56.21383	-20.63171	17.25549	-9.37870
-3.44901	55.56560	-97.27793	86.51073	-41.88848	20.53830
2.11302	-13.11647	86.94411	-230.47475	235.64856	-81.11407
-3.91735	20.34595	-78.08396	437.12418	-1716.64771	1341.18115
-15.17317	75.14519	-253.82050	915.66913	-2866.75830	2144.94092

Six Interior Collocation Points

THE COLLOCATION POINTS ARE

0.23046E+00 0.44849E+00 0.64235E+00 0.80158E+00 0.91760E+00 0.98418E+00
0.10000E+01

A:

-6.75214	12.30303	-11.22067	12.06122	-14.46644	21.33112	-13.25591
-1.53348	-3.90577	9.39463	-7.93257	8.77009	-12.53088	7.73808
0.40832	-2.74294	-3.42855	9.84743	-8.46474	11.18572	-6.80532
-0.17615	0.92981	-3.95517	-4.11522	12.90452	-13.50796	7.92048
0.09383	-0.45656	1.50988	-5.73102	-7.44179	24.80138	-12.77456
-0.05075	0.23970	-0.73180	2.19961	-9.08694	-32.88064	40.30906
0.07765	-0.36353	1.09387	-3.16797	11.50732	-99.14404	89.99902

B:

-55.08609	70.62412	-23.30976	12.98954	-9.86146	11.09597	-6.45018
20.30436	-74.29181	69.14916	-23.33082	14.69621	-15.20988	8.68210
-3.81016	39.32206	-104.22478	88.50545	-32.12555	27.20430	-14.86842
1.75009	-10.93231	72.91641	-176.56384	149.54562	-72.21495	35.50605
-1.53010	7.92972	-30.46669	172.04152	-430.40671	430.81384	-148.36337
3.40943	-16.24978	51.06896	-164.37776	852.13965	-3254.39941	2528.38965
13.87886	-64.69531	192.83655	-544.45508	1814.63037	-5507.16357	4094.97266

APPENDIX B

SPEEDUP™ IX MODEL OF A CST THREE-COLUMN CAROUSEL

The CST IX process is schematically represented by the SpeedUp flowsheet shown in Figure B1. The entire model consists of six units: feeder, IX1, IX2, IX3, decon_product, and cst_info. IX1, IX2 and IX3 are physical units representing the three CST IX columns. Feeder, CST_Info and Decon_Product are non-physical units used for information extraction and conversion of chemical component vector. Brief description of each unit is given below.

Figure B1: Schematic SpeedUp™ Flow Diagram of the CST IX Process

<u>Unit</u>	<u>Description</u>
Feeder	Combine the salt solution and utility streams to a single feed stream to the first CST IX column, and convert the 51-component feed stream into a 2-component stream.
IX1	Model the CST IX first (lead) column. IX1 is a macro consisting of STAGE and MONITOR submodels. STAGE computes the material balance in a column element of length dz. MONITOR provides data at the column exit (i.e. relative Cs concentration df, Cs mass concentration, and Cs amount adsorbed on CST bed)
IX2	Model the CST IX second column. Functions similar to IX1.
IX3	Model the CST IX third (guard) column. Functions similar to IX1 and IX2.
Decon_Product	Convert the 2-component product stream at the outlet of the third IX column back to a 51-component decontaminated salt solution stream.

CST_Info

Provide information about the 10 Wt% CST slurry to be sent to DWPF. The slurry is resulted from treatment of the loaded CST resin in the lead column taken out of service at the end of a cycle. In addition to the slurry information, cycle time and total Cs loading are also given.

The CST IX process is operated as follows (Beck et al., 1998). The standard three-column carousel arrangement is assumed. This arrangement includes a lead (first) column followed by a middle (second) column and a guard (third) column to assure sufficient decontamination. A fourth column is maintained standby loaded with fresh resin. A cycle is completed when the Cs concentration in the liquid at the exit of the second column reaches 1.3 micrograms Cs/L (or 20 nCi/g). At the end of the cycle, the close-to-saturation (expected to be > 90%) loaded lead column is taken out of service, the second column becomes the lead column, the third column becomes the middle column and the fresh, standby column becomes the third, or, guard column. The resin is slurried from the loaded column, fresh resin is added, and this column then goes to standby.

The column switching at the end of a cycle is simulated in SpeedUp™ by utilizing the INITIAL subsection of the OPERATION section. To initialize each run, three types of variables are required in each column: Cs amount loaded on CST resin, bulk-phase Cs concentration, and pore-phase Cs concentration. At the beginning of the first cycle, all these variables assume zero values. At the end of a cycle, the computed values of these variables are captured for columns 2 and 3. In the next cycle, the values in column 2 from the previous cycle are used for those in column 1, and the values in column 3 become those in column 2. The variables in column 3 are set to zero since the new standby column is loaded with fresh resin. The REPORT OPERATION_50 (for 50 axial elements/column) and REPORT OPERATION_100 (for 100 axial elements/column) are used to capture the values of all these variables at the end of a cycle and to create the new OPERATION section to be used in the next cycle.

Design Case

A design case is to be run to determine the cycle time. Data required for the run are summarized below:

Salt feed rate:	21.1 gal/min
Na+:	5.60 M
Density:	10.5 lbs/gal
Feed rate:	20.1 gal/min
Na+:	5.60 M
Density:	10.5 lbs/gal
Mass fraction:	

H ₂ O	0.716378809
Misc. Na ⁺ salts	0.006222338
NaNO ₃	0.133755585
NaNO ₂	0.026269631
NaOH	0.071438676

NaAlO ₂	0.018277153
CsOH	1.65322E-05
KOH	0.00063232
Na ₂ CO ₃	0.012030905
Na ₂ SO ₄	0.01497805

Column length: 16 ft
Column diameter: 5 ft
CST bed void: 0.5
CST particle void: 0.26
Particle diameter: 375 μ m
Particle diffusivity: 5×10^{-5} cm²/min
Langmuir isotherm: a = 2562 ml/ml B.V.
b = 33.26 ml/mg

Results

The REPORT SUMMARY captures the specified and computed data to provide the following outputs:

1. The salt solution feed stream.
2. Utility streams (water and NaOH).
3. Decontaminated salt solution.
4. CST slurry stream.
5. CST cycle time.
6. Loading of Cesium on CST (mg Cs/g CST) in the CST slurry.
7. Profile of Cs concentration in the liquid phase along the entire length of the three columns.

The result shows that Cesium is practically removed within the first two columns. Very small amount of Cesium reaches the third column. Due to the fresh resin loaded in the lead column at the start of the operation, the cycle time is longer in the first cycle (3950 hours), then approaches a stable value in subsequent cycles (~ 2945 hours). The complete result of the analysis is shown below in Table B1.

Table B1: Result of Cycle 1 / Design Case

CASE:	DESIGNCASE
Cycle Number:	CYCLE1
Cycle Time (hrs):	3950.16144
Column Diameter (ft):	5.00000
Column Length (ft):	16.00000
Salt Feed Stream (Including Water and NaOH additions):	
Flow rate (gpm):	21.10000


```
0.12031E-1
0.14978E-1
```

1. H2O
2. Misc. salts
3. NaNO3
4. NaNO2
5. NaOH
6. KNO3
7. CsNO3
8. NH4NO3
9. NH4OH
10. NaAlO2
11. Misc. sludge
12. Na2U2O7
13. Fe(OH)3
14. Al(OH)3
15. Cr(OH)2
16. C6H6
17. Phenol/Phenoxide
18. CsOH
19. KOH
20. CsB(C6H5)4
21. NaB(C6H5)4
22. Na2(C6H5)BO2
23. KB(C6H5)4
24. NH4B(C6H5)4
25. NaTi2O5H
26. NaT.S(OH)2
27. NaT.Na2U2O7
28. (C6H5)3B
29. (C6H5)2BOH
30. (C6H5)B(OH)2
31. B(OH)3
32. K2O
33. LiO2
34. MO
35. MnO
36. TiO2
37. U3O8
38. ZrO2
39. Ca3P2O8
40. P2O5
41. Cr2O3
42. CsO2
43. CuO
44. Na2O
45. NiO
46. SiO2
47. HgO
48. alpha (PuO2)
49. CaCO3
50. Na2CO3
51. Na2SO4

Additions to Salt Feed Stream:

Water to load CST (gals):
2M NaOH solution (gals):

47100.
23500.

CST Slurry Stream per Cycle:

Solid CST (lbs): 19601.90831
Cs (lbs): 574.47351
Water (lbs): 181587.43636

Loading of Cs on solid CST (mg Cs/g CST): 29.30702

Cs Concentration (mol/L) in the Salt Solution along Column 1
(Values given at equal distance between inlet and outlet)

Inlet: 0.13877E-3
0.13877E-3
0.13877E-3
0.13876E-3
0.13876E-3
0.13876E-3
0.13876E-3
0.13876E-3
0.13873E-3
0.13856E-3
Outlet: 0.13774E-3

Cs Concentration (mol/L) in the Salt Solution along Column 2
(Values given at equal distance between inlet and outlet)

Inlet: 0.13774E-3
0.13403E-3
0.12028E-3
0.86755E-4
0.43318E-4
0.14810E-4
0.40095E-5
0.97468E-6
0.22247E-6
0.47980E-7
Outlet: 0.97818E-8

Cs Concentration (mol/L) in the Salt Solution along Column 3
(Values given at equal distance between inlet and outlet)

Inlet: 0.97818E-8
0.18512E-8
0.32696E-9
0.0
0.0
0.0
0.0
0.0
0.0
0.0
Outlet: 0.0

Model Listing

A full listing of the SpeedUp™ Ion Exchange model of a CST three-column carousel will be provided on the pages following. In addition, an electronic copy is available on the RS/6000 cluster in the directory file:

`/.../dce.srs.gov/fs/user/t8429/ix/cst_ix/bcase_50.speedup`

TITLE

```

CST Ion Exchange Model for A Three-Column Carousel
#####
# Author:                                     #
#                                           #
#           T. Hang & R. A. Dimenna          #
#                                           #
#           Westinghouse Savannah River Company      #
#                                           #
#           Version of 28 September 1999            #
#                                           #
#####
#           THIS SOFTWARE WAS DEVELOPED UNDER WSRC'S      #
#           MANAGEMENT AND OPERATIONS CONTRACT          #
#           NO. DE-AC09-89SR18035.  WSRC AND DOE        #
#           RESERVE ALL RIGHTS.                        #
#####

```

OPTIONS

```

Routines
  Superdae
Execution
  PRINTLEVEL = 1
  TARGET      = TERMINAL
  TIME_STEP   = 10
  ABS_TOL     = 1e-7
  REL_TOL     = 1e-5
  EVENT_TOL   = 1e-5
  INTERVALS   = 600
  BOUNDCHECK  = OFF

```

DECLARE

Type

#	Variable name	Initial	Minimum	Maximum	Units of measurement
	AREA	= 1.0	: 0.0	: 100.0	UNIT = "m2"
	COEFF	= 0.0	: -100.0	: 100.0	UNIT = "m2"
	CONCENTRATION	= 0.0	: 0.0	: 100.0	UNIT = "moles/l"
	CONC2	= 0.0	: 0.0	: 1.0	UNIT = "moles/l"
	DENSITY	= 0.0	: 0.0	: 2000.0	UNIT = "kg/m3"
	DENSITY2	= 10.0	: -1E-3	: 1E3	UNIT = "LB/GAL"
	FLOWRATE	= 1.0	: -1E-3	: 1E5	UNIT = "KGAL/DAY"
	LENGTH	= 0.0	: 0.0	: 100.0	UNIT = "m"
	MASS	= 1.0	: -1E3	: 1E7	UNIT = "lbs"
	MASSFRAC	= 0.0	: 0.0	: 1.0	UNIT = " "
	MASSCONC	= 0.0	: -1E3	: 1E3	UNIT = "G/L"
	MOLFLOW	= 0.0	: -1E3	: 1E10	UNIT = "moles/hr"
	MOLFRAC	= 0.0	: 0.0	: 1.0	UNIT = " "
	MOLTRANRATE	= 1.0	: 0.0	: 1.e7	UNIT = "mole/hr-m3"
	MOLWEIGHT	= 1.0	: 0.0	: 1000.0	UNIT = "g/mole"
	NUNIT	= 0.0	: -0.0001	: 100.0	UNIT = " "
	NUNIT2	= 0.0	: -1E-3	: 1E6	UNIT = " "
	Percent_MF	= 0.0	: 0.0	: 100.0	UNIT = " "
	TEMPERATURE	= 40.	: -1E-3	: 1E3	UNIT = "DEG-C"
	TIME	= 0.0	: -1E-3	: 1E4	UNIT = "hrs"
	VOLFLOW	= 1.0	: 0.0	: 1000.0	UNIT = "m3/hr"
	VOLUME	= 1.0	: 0.0	: 1E6	UNIT = "gals"

Stream MAINSTREAM

Set

NOCOMP = 51

Type

```

#Info in stream between units: flow, density, massfractions (vector)#
FLOWRATE, DENSITY2, NOUNIT(NOCOMP)

Stream LIQUID
Set
    LIQCOMP = 2
Type
    VOLFLOW, CONCENTRATION(LIQCOMP)
****
PROCEDURE PHYSP # Properties data base #
    INPUT temperature
    OUTPUT molweight(nocomp), density2(nocomp)
CODE
    SUBROUTINE physp(t,
+                wm,nocomp,dens,ncp,
+                ifail,ityp)
C
C    Revised: 5 May 1998 - added species (M.V. Gregory)
C
C Physical property database
C References: 1. CRC's Handbook Chemistry and Physics, 68th Edition
C             2. Alex Choi's DWPF CEPS Model
C
C Input: Temperature (C)
C
C Output: Mol. wt, density (lb/gal)
C
C Note: Since SpeedUp's PROCEDURE requires at least an input variable,
C       temperature is used as a dummy input variable only.
C
C Components:
C 1 H2O
C 2 Miscellaneous salts
C 3 Sodium nitrate NaNO3
C 4 Sodium nitrite NaNO2
C 5 Sodium hydroxide NaOH
C 6 Potassium nitrate KNO3
C 7 Cesium nitrate CsNO3
C 8 Ammonium nitrate NH4NO3
C 9 Ammonium hydroxide NH4OH
C 10 NaAlO2
C 11 Miscellaneous sludge
C 12 Na2U2O7
C 13 Fe(OH)3
C 14 Al(OH)3
C 15 Cr(OH)2
C 16 Benzene C6H6
C 17 Phenol/Phenoxide
C 18 Cesium hydroxide CsOH
C 19 Potassium hydroxide KOH
C 20 Cesium TPB CsB(C6H5)4
C 21 Sodium TPB NaB(C6H5)4
C 22 Sodium phenylboronate Na2(C6H5)BO2
C 23 Potassium TPB KB(C6H5)4
C 24 Ammonium TPB NH4B(C6H5)4
C 25 Sodium titanate NaTi2O5H
C 26 NaT.Sr(OH)2
C 27 NaT.Na2U2O7
C 28 Triphenylboron (C6H5)3B
C 29 Diphenylboronic acid (C6H5)2BOH
C 30 Phenylboronic acid (C6H5)B(OH)2
C 31 Boric acid B(OH)3
C 32 K2O

```

C 33 LiO2
C 34 MO
C 35 MnO
C 36 TiO2
C 37 U3O8
C 38 ZrO2
C 39 Ca3P2O8
C 40 P2O5
C 41 Cr2O3
C 42 CsO2
C 43 CuO
C 44 Na2O
C 45 NiO
C 46 SiO2
C 47 HgO
C 48 alpha (PuO2)
C 49 CaCO3
C 50 Na2CO3
C 51 Na2SO4
C

IMPLICIT DOUBLE PRECISION (a-h,o-z)
DIMENSION wm(nocomp), dens(ncp), rho(51), wtmol(51)

C
C=====table of molecular weights - grams/mole ("99.999" are dummies)
C parallels structure of mainstream vector plus partial components
C added to end of table.
C

data wtmol /			
&	18.01534	, 99.999	! H2O , miscellaneous salts
&	84.9947	, 68.9953	! NaNO3 , NaNO2
&	39.99717	, 101.1069	! NaOH , KNO3
&	194.9099	, 80.04348	! CsNO3 , NH4NO3
&	35.04595	, 81.9701	! NH4OH , NaAlO2
&	99.999	, 634.0354	! miscellan sludge, Na2U2O7
&	106.86911	, 78.00361	! Fe(OH)3 , Al(OH)3
&	121.63474	, 78.11472	! Sr(OH)2 , Benzene
&	93.61014	, 149.91237	! Phenol/Phenoxide, CsOH
&	56.10937	, 452.143	! KOH , CsTPB
&	342.2278	, 165.89615	! NaTPB , NaDTB
&	358.34	, 337.27658	! KTPB , NH4TPB
&	199.79477	, 321.42951	! NaTitanate , NaT.Sr(OH)2
&	833.83017	, 242.13	! NaT.Na2U2O7 , (C6H5a)3B
&	181.81	, 121.93	! (C6H5)2BOH , (C6H5)B(OH)2
&	61.83	, 94.203	! B(OH)3 , K2O
&	29.877	, 40.311	! LiO2 , MgO
&	70.937	, 79.899	! MnO , TiO2
&	842.085	, 123.219	! U3O8 , ZrO2
&	310.183	, 141.945	! Ca3P2O8 , P2O5
&	151.99	, 291.809	! Cr2O3 , Cs2O
&	79.539	, 61.979	! CuO , Na2O
&	74.709	, 60.085	! NiO , SiO2
&	216.589	, 271.129	! HgO , alpha (PuO2)
&	100.089	, 106.	! CaCO3 , Na2CO3
&	142.04		! Na2SO4
&			

C
C=====table of specific gravities,
C parallels structure of mainstream vector
C

data rho /			
&	1.	, 2.477	! H2O , miscellaneous salts
&	2.261	, 2.168	! NaNO3 , NaNO2
&	2.13	, 2.109	! NaOH , KNO3

```

& 3.685 , 1.725 , ! CsNO3 , NH4NO3
& 1.2 , 2.183 , ! NH4OH , NaAlO2
& 3.0 , 3.148 , ! miscellan sludge, Na2U2O7
& 3.4 , 2.42 , ! Fe(OH)3 , Al(OH)3
& 3.625 , 0.8765, ! Sr(OH)2 , Benzene
& 1.058 , 3.675 , ! Phenol/Phenoxide, CsOH
& 2.044 , 1.483 , ! KOH , CsTPB
& 1.199 , 1.276 , ! NaTPB , NaDTB
& 1.276 , 0.996 , ! KTPB , NH4TPB
& 2.765 , 2.765 , ! NaTitanate , NaT.Sr(OH)2
& 2.765 , 1. , ! NaT.Na2U2O7 , (C6H5)3B
& 1. , 1. , ! (C6H5)2BOH , (C6H5)B(OH)2
& 1.435 , 2.32 , ! B(OH)3 , K2O
& 2.013 , 3.615 , ! LiO2 , MgO
& 5.31 , 4.09 , ! MnO , TiO2
& 7.8 , 5.68 , ! U3O8 , ZrO2
& 3.14 , 2.387 , ! Ca3P2O8 , P2O5
& 5.21 , 4.25 , ! Cr2O3 , Cs2O
& 6.03 , 2.27 , ! CuO , Na2O
& 7.06 , 2.29 , ! NiO , SiO2
& 11.1 , 11.46 , ! HgO , alpha (PuO2)
& 2.93 , 2.533 , ! CaCO3 , Na2CO3
& 2.698 , ! Na2SO4
& /

C
C=====reference density of H2O, lbm/gal
C
data water_rho /8.3454/
dummy = t
DO 5 I = 1,51
dens(i) = water_rho * rho(i)
wm(i) = wtmol(i)
5 CONTINUE
ifail = 1
RETURN
END
$ENDCODE
****
PROCEDURE SYM_COLL # ORTHOGONAL COLLOCATION #
INPUT concentration(npoint), concentration
OUTPUT nounit2(npoint), nounit2
CODE
SUBROUTINE sym_coll(c_pa,npoint,c_A0,
+ d2cpAdr2,npt,dcpAdr,
+ ifail,ityp)
C
C ORTHOGONAL COLLOCATION APPLIED TO SYMMETRIC FUNCTION IN
C SPHERICAL COORDINATES WITH WEIGHTING FUNCTION W = 1
C (SOURCE: "NONLINEAR ANALYSIS IN CHEMICAL ENGINEERING"
C B.A. FINLAYSON, MCGRAW-HILL, 1980
C TABLE 4-5
C
C IMPLICIT DOUBLE PRECISION (a-h,o-z)
C DIMENSION c_pa(npoint),d2cpadr2(npt)
C
C SECOND DERIVATIVE @ 3 INTERIOR COLLOCATION POINTS
C (r/R) = 0.40585, 0.74153 and 0.90618
C
d2cpAdr2(1) = - 20.02574*c_pa(1) + 26.60195*c_pa(2)
+ - 12.57212*c_pa(3) + 5.99591*c_A0
d2cpAdr2(2) = 10.87790*c_pa(1) - 44.91904*c_pa(2)
+ + 51.74983*c_pa(3) - 17.70865*c_A0
d2cpAdr2(3) = - 6.77880*c_pa(1) + 68.23693*c_pa(2)

```



```

+          -313.05557*c_pA(3) +251.59755*c_A0
C
C FIRST DERIVATIVE AT (r/R) = 1
C
      dcpAdr = - 0.37710*c_pA(1) + 2.72364*c_pA(2)
+      -29.34654*c_pA(3) + 27*c_A0
      ifail = 1
      RETURN
    END
$ENDCODE
****
MODEL      CST_INFO
#
# Provide information about the 10 Wt% CST slurry stream going to DWPF      #
#=====#
#   Author:          T. Hang, SRTC                                         #
#   Version Date: 29 September 1998                                       #
#=====#
#
SET
  PI = 3.1415927,
  Cs_MW = 132.9          # Cs Mol. Weight #

TYPE
  CsNO3_conc, CsOH_conc          AS CONCENTRATION
  CST_bulk_density, H2O_density  AS DENSITY2
  Cs_mass, Cs_mass_IX1, CST_mass, H2O_mass  AS MASS
  column_diameter, column_length  AS LENGTH
  CST_volume, H2O_volume          AS VOLUME
  Wt_percent, DF                 AS NOUNIT
  cycle_time, time              AS TIME

STREAM
  CONNECTION 1 IS DF
  CONNECTION 2 IS CsNO3_conc, CsOH_conc

EQUATION
#
# Total mass of CST
#
      CST_volume = (PI/4) * column_diameter^2 * column_length * (7.48*35.3);
      CST_mass = CST_volume * CST_bulk_density;
#
# Water amount to slurry CST to 10 Wt%
#
      Wt_percent = 10.;
      H2O_density = 8.345;
      H2O_mass = H2O_volume * H2O_density;
      Wt_percent * (CST_mass + Cs_mass + H2O_mass) = (CST_mass + Cs_mass) * 100.;
#
# Total Cs amount adsorbed on CST solids and trapped
# in CST pores
#
      Cs_mass = Cs_mass_IX1;
#
# Cycle time
#
      cycle_time = time;
****
MODEL      DECON_PRODUCT
#
# Convert the 2-component IX outlet stream back into the 51-component      #
# decontaminated salt solution stream                                       #

```

```

=====
# Author:      T. Hang, SRTC                                     #
# Version Date: 29 September 1998                               #
=====
# Model Connectivity:                                           #
#                                                           #
#               -----                                         #
# 1. Input      --->|           |---> 1. Output               #
#   (IX Outlet stream) ----- (Decon Salt Stream)             #
=====
#
SET
nocomp,      # 51 components #
liqcomp,     # 2 components #
      # chemical component vector specific ID's #
CsNO3,
CsOH,
CsNO3b,
CsNO3a,
CsOHb,
CsOHa

TYPE
in_flow      AS VOLFLOW
in_molflow   AS MOLFLOW
out_flow     AS FLOWRATE
in_conc, out_conc AS CONCENTRATION
c_init, c_final AS CONCENTRATION
rho_solvent  AS DENSITY
out_density, feed_density AS DENSITY2
MW_out, MW_solvent AS MOLWEIGHT
df           AS NOUNIT
CsOH_ratio, CsNO3_ratio AS NOUNIT2
in_temp      AS TEMPERATURE
out_comp_conc, feed_conc AS ARRAY(NOCOMP) OF CONCENTRATION
in_comp_conc AS ARRAY(LIQCOMP) OF CONCENTRATION
density, dummy_density AS ARRAY(NOCOMP) OF DENSITY2
out_molfrac  AS ARRAY(NOCOMP) OF MOLFRAC
in_molfrac   AS ARRAY(LIQCOMP) OF MOLFRAC
out_massfrac AS ARRAY(NOCOMP) OF NOUNIT
molfrac_MW   AS ARRAY(NOCOMP) OF NOUNIT2
wm           AS ARRAY(NOCOMP) OF MOLWEIGHT

STREAM
OUTPUT 1 IS out_flow, out_density, out_massfrac
INPUT 1 IS in_flow, in_comp_conc

EQUATION
#
# Dummy temperature
#
in_temp = 35.;
#
# Dummy density
#
dummy_density = density;
#
# Total decontamination factor
#
df * c_init = c_final;
#
# Inlet mole fraction

```

```

#
in_conc = SIGMA(in_comp_conc);
in_molfrac * in_conc = in_comp_conc;
#
# Reduction in Cs molar concentration
#
out_comp_conc(CsNO3) = feed_conc(CsNO3) * df * CsNO3_ratio;
out_comp_conc(CsOH) = feed_conc(CsOH) * df * CsOH_ratio;
out_comp_conc(1:CsNO3b) = feed_conc(1:CsNO3b);
out_comp_conc(CsNO3a:CsOHb) = feed_conc(CsNO3a:CsOHb);
out_comp_conc(CsOHa:nocomp) = feed_conc(CsOHa:nocomp);
out_conc = SIGMA(out_comp_conc);
#
# Mole fraction and mass fraction
#
out_molfrac * out_conc = out_comp_conc;
molfrac_MW = out_molfrac * wm;
out_massfrac * SIGMA(molfrac_MW) = out_molfrac * wm;
#
# MW
#
MW_out = SIGMA(molfrac_MW);
MW_solvent = MW_out * in_molfrac(1);
#
# Density
#
out_density = feed_density;
rho_solvent = out_density * 119.8322;
#
# Convert m3/hr (Solvent) to mol/hr (Total)
#
in_molflow * MW_solvent * in_molfrac(1) = in_flow * rho_solvent * 1000;
#
# Convert mole flow rate (mol/hr) to volumetric flow rate (kgal/day)
#
out_flow * out_density * 18900 = in_molflow * MW_out;

PROCEDURE
(wm, density) PHYSP (in_temp)
  # Get component mol. wt. and density      #
  # Note: in_temp is dummy input variable #
****
MODEL      FEEDER
#
# Combine different streams to a single feed stream to CST IX column and      #
# convert the 51-component feed stream into a 2-component stream              #
#=====
#   Author:      T. Hang, SRTC                                              #
#   Version Date: 30 September 1998                                         #
#=====
#   Model Connectivity:
#
#
#   1. Salt Solution      ---->|          |----> 1. Output
#   2. Inventory water    ---->|          |
#   3. 2M NaOH            ---->|          |
#   4. Excess water       ---->|          |
#
#=====
#
SET
nocomp,      # 51 components #
liqcomp,     # 2 components #

```

```

# chemical component vector specific ID's #
CsNO3,
CsOH
#
TYPE
  in1_flow, in2_flow, in3_flow, in4_flow, in_flow      AS FLOWRATE
  in1_density, in2_density, in3_density, in4_density,
  in_density                                           AS DENSITY2
  rho_solvent, out_density                             AS DENSITY
  in_conc, out_conc, CsNO3_conc, CsOH_conc            AS CONCENTRATION
  in_temp                                              AS TEMPERATURE
  out_flow                                             AS VOLFLOW
  in_molflow, out_molflow                             AS MOLFLOW
  MW_in, MW_solvent                                   AS MOLWEIGHT
  CsOH_ratio, CsNO3_ratio                             AS NOUNIT2
  in_comp_conc                                         AS ARRAY(NOCOMP) OF CONCENTRATION
  density, dummy_density                             AS ARRAY(NOCOMP) OF DENSITY2
  out_comp_conc                                       AS ARRAY(LIQCOMP) OF CONCENTRATION
  out_molfrac                                         AS ARRAY(LIQCOMP) OF MOLFRAC
  in_molfrac                                           AS ARRAY(NOCOMP) OF MOLFRAC
  in_massfrac, in1_massfrac, in2_massfrac,
  in3_massfrac, in4_massfrac, MW_in_comp              AS ARRAY(NOCOMP) OF NOUNIT
  out_massfrac                                         AS ARRAY(LIQCOMP) OF NOUNIT
  massfrac2wm_comp_ratio                             AS ARRAY(NOCOMP) OF NOUNIT2
  wm                                                   AS ARRAY(NOCOMP) OF MOLWEIGHT
#
STREAM
  OUTPUT 1 IS out_flow, out_comp_conc
  INPUT 1 IS in1_flow, in1_density, in1_massfrac
  INPUT 2 IS in2_flow, in2_density, in2_massfrac
  INPUT 3 IS in3_flow, in3_density, in3_massfrac
  INPUT 4 IS in4_flow, in4_density, in4_massfrac
  CONNECTION 1 IS CsNO3_conc, CsOH_conc
#
EQUATION
#
# Set dummy temperature
#
  in_temp = 35.;
#
# Set dummy density
#
  dummy_density = density;
#
# Assuming that volumes are just added
#
  in_flow = in1_flow + in2_flow + in3_flow + in4_flow;
#
# Overall mass balance
#
  in_flow * in_density =
    in1_flow * in1_density + in2_flow * in2_density +
    in3_flow * in3_density + in4_flow * in4_density;
#
# Component mass balance
#
  in_flow * in_density * in_massfrac =
    in1_flow * in1_density * in1_massfrac +
    in2_flow * in2_density * in2_massfrac +
    in3_flow * in3_density * in3_massfrac +
    in4_flow * in4_density * in4_massfrac;
#
# Convert mass fraction to mole fraction

```

```

#
massfrac2wm_comp_ratio * wm = in_massfrac;
in_molfrac * wm * SIGMA(massfrac2wm_comp_ratio) = in_massfrac;
#
# Convert density from lb/gal to kg/m3
#
out_density = in_density * 119.8322;
#
# Total MW
#
MW_in_comp = wm * in_molfrac;
MW_in = SIGMA(MW_in_comp);
#
# Molar concentration
#
in_conc * MW_in = 119.84 * in_density;
in_comp_conc = in_molfrac * in_conc;
CsNO3_conc = in_comp_conc(CsNO3);
CsOH_conc = in_comp_conc(CsOH);
#
# Convert mass flow rate to mole flow rate
#
in_molflow * MW_in = in_flow * in_density * 18900;
#
# Construct the 2-component stream
#
out_flow * rho_solvent =
  in_flow * out_massfrac(1) * 0.1578 * out_density; # Solvent vol. flow
out_molflow = in_molflow * out_molfrac(1); # Solvent mole flow
out_molfrac(1) = 1 - out_molfrac(2); # Solvent mole frnx
out_molfrac(2) = in_molfrac(CsNO3) + in_molfrac(CsOH); # Cs mole frxn
out_massfrac(1) = 1 - out_molfrac(2); # Solvent mass frxn
out_massfrac(2) = in_massfrac(CsNO3) + in_massfrac(CsOH); # Cs mass frxn
rho_solvent * (1/in_density -
  in_massfrac(CsNO3)/density(CsNO3) -
  in_massfrac(CsOH)/density(CsOH)) =
  out_massfrac(1) * 119.8322; # Solvent density
MW_solvent = MW_in * out_molfrac(1); # Solvent MW
out_conc = in_conc; # Molar density
out_comp_conc = out_molfrac * out_conc; # Comp. molar conc.
CsNO3_ratio * out_molfrac(2) = in_molfrac(CsNO3);
CsOH_ratio * out_molfrac(2) = in_molfrac(CsOH);

```

PROCEDURE

```

(wm, density) PHYSP (in_temp)
# Get component mol. wt. and density #
# Note: in_temp is dummy input variable #

```

MODEL Monitor

Set

```

LIQCOMP,
Cs_MW = 132.9

```

Type

```

in_conc, out_conc, c_init as CONCENTRATION
Cs_mass as MASS
Cs_massconc as MASSCONC
W_in as MOLFLOW
df as NUNIT
x_init as MOLFRAC
in_comp_conc, out_comp_conc as ARRAY(LIQCOMP) OF CONCENTRATION
x_in, x_out as ARRAY(LIQCOMP) OF MOLFRAC

```

```

Flow_in, Flow_out          as VOLFLOW

Stream
  Input      1 is FLOW_in,  in_comp_conc
  Output     1 is FLOW_out, out_comp_conc
  Connection 1 is df

Equation

# Set outlet stream equal to inlet stream

  Flow_in = Flow_out;
  in_comp_conc = out_comp_conc;
  in_conc = SIGMA(in_comp_conc);
  out_conc = in_conc;
  x_in * in_conc = in_comp_conc;
  x_out = x_in;

# Calculate the df for the column

  if x_out(2) > 1e-10 then
    df * c_init = out_comp_conc(2)
  else
    df = 0
  endif;

# Cs mass concentration at the column outlet

  Cs_massconc = out_comp_conc(2) * Cs_MW;
#
# Cs amount adsorbed on CST
#
  $Cs_mass * 453.59 = (1-df) * x_init * W_in * Cs_MW;
****
MODEL STAGE
#
#                               Model of Single Element of IX Column                               #
#=====
#   Author:      R.A. Dimenna, SRTC                                     #
#   Version Date: 24 July 1998                                         #
#=====
#   Modification History:
#   Mod No.   Date   Author   Description
#   -----
#       01    11/04/98   T. Hang   Add axial dispersion and pore diffusion
#       02    01/28/99   T. Hang   Orth. collocation for pore diffusion
#       03    02/04/99   T. Hang   Orth. collocation for axial elements
#=====
#   Model Connectivity:
#
#
#   1. Input      ---->|      IX      |----> 1. Output
#   (Element n-1) | (Element n) | (Element n+1)
#
#=====
#
Set
  LIQCOMP,          # 1: Solvent, 2: Solute #
  NZ = 3,           # No. of coll. points in each axial element #
  NP = 4            # No. of interior coll. points in the particle #

Type
  S                  as AREA

```

```

c_A_in, c_A_out, c_A0_out      as CONCENTRATION
in_conc, out_conc              as CONCENTRATION

rho_solvent                    as DENSITY

deltaZ, diameter, R            as LENGTH

W_B, W_csIn, Wm_solid,
W_in                           as MOLFLOW
W_out, W_csOut                 as MOLFLOW

in_comp_conc, out_comp_conc    as ARRAY(LIQCOMP) OF CONCENTRATION
c_A, c_A0                     as ARRAY(NZ) OF CONCENTRATION
c_pA1, c_pA2, c_pA3, c_pA_out as ARRAY(NP) OF CONCENTRATION
x_in, x_out                    as ARRAY(LIQCOMP) OF MOLFRAC

MW_solvent                     as MOLWEIGHT

epsilon, kf, disp_coeff,
diff_coeff, eps_p              as NOUNIT
velocity                       as NOUNIT
Stage_No, NELEM, iso_a, iso_b  as NOUNIT2
dcpA1sdcpA1, dcpA2sdcpA2,
dcpA3sdcpA3, dcpAoutsdcpAout  as ARRAY(NP) OF NOUNIT2

FLOW_out, FLOW_in              as VOLFLOW

```

Stream

```

Input 1 is FLOW_in, in_comp_conc

Output 1 is FLOW_out, out_comp_conc

```

Equation

```

#
# Inlet and outlet concentrations and mole fractions
#
in_conc = SIGMA(in_comp_conc);
out_conc = SIGMA(out_comp_conc);
x_in * in_conc = in_comp_conc;
x_out * out_conc = out_comp_conc;
#
# Set up the input flow rates
#
W_B * MW_solvent = Flow_in * rho_solvent * 1000.;

if x_in(1) <= 0 then
    W_in = W_B
else
    W_in * x_in(1) = W_B
endif;

W_csIn = W_in - W_B;
#
# Interstitial velocity
# Note: Interstitial vel. = Superficial vel. / Void
#                      = (F / S) / epsilon
#
Velocity * epsilon * S = Flow_in;
#
# Mass balance
#
Flow_in = Flow_out; #This balance ensures that solvent is

```

```

#conserved.
#
# Component mass balances
#
# Bulk phase #

# Use of orthogonal collocation
# Select 3 interior collocation points at  $x = (z/\text{deltaZ}) = 0.11270$ ,
# 0.5, and 0.88730
# Hence:
# c_A(1): Bulk-phase solute conc. @  $x = 0.11270$ 
# c_A(2): Bulk-phase solute conc. @  $x = 0.5$ 
# c_A(3): Bulk-phase solute conc. @  $x = 0.88730$ 

If Stage_No = 1 then
  (-13*c_A_in + 14.78830*c_A(1) - 2.66667*c_A(2) + 1.87836*c_A(3)
   - 1.0*c_A_out) =
    (velocity*deltaZ/disp_coeff) * (c_A_in - in_comp_conc(2))
else
  c_A_in = in_comp_conc(2)
endif;

$c_A(1) =
  - (velocity/deltaZ) *
    (-5.32379*c_A_in + 3.87298*c_A(1) + 2.06559*c_A(2) - 1.29099*c_A(3)
     + 0.67621*c_A_out)
  + (disp_coeff/deltaZ^2) *
    (53.23790*c_A_in - 73.33334*c_A(1) + 26.66667*c_A(2) -
     13.33334*c_A(3) + 6.76210*c_A_out)
  - (6.*kf/diameter) * ((1-epsilon)/epsilon) * (c_A(1)-c_A0(1));

$c_A(2) =
  - (velocity/deltaZ) *
    (1.5*c_A_in - 3.22749*c_A(1) + 0.0*c_A(2) + 3.22749*c_A(3) -
     1.5*c_A_out)
  + (disp_coeff/deltaZ^2) *
    (-6.0*c_A_in + 16.66667*c_A(1) - 21.33334*c_A(2) + 16.66667*c_A(3) -
     6.0*c_A_out)
  - (6.*kf/diameter) * ((1-epsilon)/epsilon) * (c_A(2)-c_A0(2));

$c_A(3) =
  - (velocity/deltaZ) *
    (-0.67621*c_A_in + 1.29099*c_A(1) - 2.06559*c_A(2) - 3.87298*c_A(3) +
     5.32379*c_A_out)
  + (disp_coeff/deltaZ^2) *
    (6.76210*c_A_in - 13.33333*c_A(1) + 26.66666*c_A(2) - 73.33334*c_A(3) +
     53.23790*c_A_out)
  - (6.*kf/diameter) * ((1-epsilon)/epsilon) * (c_A(3)-c_A0(3));

If Stage_No = NELEM then
  (1.0*c_A_in - 1.87836*c_A(1) + 2.66667*c_A(2) - 14.78831*c_A(3) +
   13*c_A_out) = 0
Else
  $c_A_out =
    - (velocity/deltaZ) *
      (1.0*c_A_in - 1.87836*c_A(1) + 2.66667*c_A(2) - 14.78831*c_A(3) +
       13*c_A_out)
    + (disp_coeff/deltaZ^2) *
      (24*c_A_in - 44.60350*c_A(1) + 58.66666*c_A(2) -
       122.06319*c_A(3) + 84*c_A_out)
    - (6.*kf/diameter) * ((1-epsilon)/epsilon) * (c_A_out-c_A0_out)
Endif;

```



```
# Particle pore diffusion #

R = 0.5 * diameter;
#
# Using Purdue's form of the Langmuir isotherm
# c_pAs * (1 + iso_b * c_pA) = iso_a * c_pA;
#
dcpA1sdcPAl * (1 + iso_b*c_pA1)'2 = iso_a;
dcpA2sdcPAl * (1 + iso_b*c_pA2)'2 = iso_a;
dcpA3sdcPAl * (1 + iso_b*c_pA3)'2 = iso_a;
dcpAoutsdcPAl * (1 + iso_b*c_pA_out)'2 = iso_a;

# Use of orthogonal collocation technique with the weighting function
# W = 1 to solve pore diffusion.
# Select 4 interior collocation points at (r/R) = 0.32425, 0.61337,
# 0.83603, and 0.96816.
# Hence:
# c_pA(1): Pore liquid-phase conc. @ (r/R) = 0.32425
# c_pA(2): Pore liquid-phase conc. @ (r/R) = 0.61337
# c_pA(3): Pore liquid-phase conc. @ (r/R) = 0.83603
# c_pA(4): Pore liquid-phase conc. @ (r/R) = 0.96816

# Particle associated with axial interior collocation point 1

(eps_p + (1.-eps_p)*dcpA1sdcPAl(1)) * $c_pA1(1) =
(eps_p*diff_coeff/R'2) *
(-29.31681*c_pA1(1) + 38.02225*c_pA1(2) - 13.89345*c_pA1(3) +
11.16665*c_pA1(4) - 5.97860*c_A0(1));

(eps_p + (1.-eps_p)*dcpA1sdcPAl(2)) * $c_pA1(2) =
(eps_p*diff_coeff/R'2) *
(12.73519*c_pA1(1) - 48.58884*c_pA1(2) + 47.69691*c_pA1(3) -
23.08930*c_pA1(4) + 11.24609*c_A0(1));

(eps_p + (1.-eps_p)*dcpA1sdcPAl(3)) * $c_pA1(3) =
(eps_p*diff_coeff/R'2) *
(-3.61367*c_pA1(1) + 37.03847*c_pA1(2) - 110.32513*c_pA1(3) +
117.18764*c_pA1(4) - 40.28716*c_A0(1));

(eps_p + (1.-eps_p)*dcpA1sdcPAl(4)) * $c_pA1(4) =
(eps_p*diff_coeff/R'2) *
(4.81349*c_pA1(1) - 29.71621*c_pA1(2) + 194.22569*c_pA1(3) -
801.76575*c_pA1(4) + 632.44220*c_A0(1));

(0.19631*c_pA1(1) - 1.10257*c_pA1(2) + 5.08667*c_pA1(3) -
48.18018*c_pA1(4) + 43.99976*c_A0(1)) =
(kf*R/eps_p/diff_coeff) * (c_A(1) - c_A0(1)); #BC @ r = R

# Particle associated with axial interior collocation point 2

(eps_p + (1.-eps_p)*dcpA2sdcPAl(1)) * $c_pA2(1) =
(eps_p*diff_coeff/R'2) *
(-29.31681*c_pA2(1) + 38.02225*c_pA2(2) - 13.89345*c_pA2(3) +
11.16665*c_pA2(4) - 5.97860*c_A0(2));

(eps_p + (1.-eps_p)*dcpA2sdcPAl(2)) * $c_pA2(2) =
(eps_p*diff_coeff/R'2) *
(12.73519*c_pA2(1) - 48.58884*c_pA2(2) + 47.69691*c_pA2(3) -
23.08930*c_pA2(4) + 11.24609*c_A0(2));

(eps_p + (1.-eps_p)*dcpA2sdcPAl(3)) * $c_pA2(3) =
(eps_p*diff_coeff/R'2) *
(-3.61367*c_pA2(1) + 37.03847*c_pA2(2) - 110.32513*c_pA2(3) +
117.18764*c_pA2(4) - 40.28716*c_A0(2));
```

```

117.18764*c_pA2(4) - 40.28716*c_A0(2));

(eps_p + (1.-eps_p)*dcpA2sdcpA2(4)) * $c_pA2(4) =
(eps_p*diff_coeff/R'2) *
(4.81349*c_pA2(1) - 29.71621*c_pA2(2) + 194.22569*c_pA2(3) -
801.76575*c_pA2(4) + 632.44220*c_A0(2));

(0.19631*c_pA2(1) - 1.10257*c_pA2(2) + 5.08667*c_pA2(3) -
48.18018*c_pA2(4) + 43.99976*c_A0(2)) =
(kf*R/eps_p/diff_coeff) * (c_A(2) - c_A0(2)); #BC @ r = R

# Particle associated with axial interior collocation point 3

(eps_p + (1.-eps_p)*dcpA3sdcpA3(1)) * $c_pA3(1) =
(eps_p*diff_coeff/R'2) *
(-29.31681*c_pA3(1) + 38.02225*c_pA3(2) - 13.89345*c_pA3(3) +
11.16665*c_pA3(4) - 5.97860*c_A0(3));

(eps_p + (1.-eps_p)*dcpA3sdcpA3(2)) * $c_pA3(2) =
(eps_p*diff_coeff/R'2) *
(12.73519*c_pA3(1) - 48.58884*c_pA3(2) + 47.69691*c_pA3(3) -
23.08930*c_pA3(4) + 11.24609*c_A0(3));

(eps_p + (1.-eps_p)*dcpA3sdcpA3(3)) * $c_pA3(3) =
(eps_p*diff_coeff/R'2) *
(-3.61367*c_pA3(1) + 37.03847*c_pA3(2) - 110.32513*c_pA3(3) +
117.18764*c_pA3(4) - 40.28716*c_A0(3));

(eps_p + (1.-eps_p)*dcpA3sdcpA3(4)) * $c_pA3(4) =
(eps_p*diff_coeff/R'2) *
(4.81349*c_pA3(1) - 29.71621*c_pA3(2) + 194.22569*c_pA3(3) -
801.76575*c_pA3(4) + 632.44220*c_A0(3));

(0.19631*c_pA3(1) - 1.10257*c_pA3(2) + 5.08667*c_pA3(3) -
48.18018*c_pA3(4) + 43.99976*c_A0(3)) =
(kf*R/eps_p/diff_coeff) * (c_A(3) - c_A0(3)); #BC @ r = R

# Particle associated with axial BC point

(eps_p + (1.-eps_p)*dcpAoutsdcpAout(1)) * $c_pA_out(1) =
(eps_p*diff_coeff/R'2) *
(-29.31681*c_pA_out(1) + 38.02225*c_pA_out(2) - 13.89345*c_pA_out(3) +
11.16665*c_pA_out(4) - 5.97860*c_A0_out);

(eps_p + (1.-eps_p)*dcpAoutsdcpAout(2)) * $c_pA_out(2) =
(eps_p*diff_coeff/R'2) *
(12.73519*c_pA_out(1) - 48.58884*c_pA_out(2) + 47.69691*c_pA_out(3) -
23.08930*c_pA_out(4) + 11.24609*c_A0_out);

(eps_p + (1.-eps_p)*dcpAoutsdcpAout(3)) * $c_pA_out(3) =
(eps_p*diff_coeff/R'2) *
(-3.61367*c_pA_out(1) + 37.03847*c_pA_out(2) - 110.32513*c_pA_out(3) +
117.18764*c_pA_out(4) - 40.28716*c_A0_out);

(eps_p + (1.-eps_p)*dcpAoutsdcpAout(4)) * $c_pA_out(4) =
(eps_p*diff_coeff/R'2) *
(4.81349*c_pA_out(1) - 29.71621*c_pA_out(2) + 194.22569*c_pA_out(3) -
801.76575*c_pA_out(4) + 632.44220*c_A0_out);

(0.19631*c_pA_out(1) - 1.10257*c_pA_out(2) + 5.08667*c_pA_out(3) -
48.18018*c_pA_out(4) + 43.99976*c_A0_out) =
(kf*R/eps_p/diff_coeff) * (c_A_out - c_A0_out); #BC @ r = R

```

```

#
# Set the outlet concentrations
#
out_comp_conc(1) = in_comp_conc(1);
out_comp_conc(2) = c_A_out;

if x_out(1) <= 0 then
    W_out = W_B
else
    W_out * x_out(1) = W_B
endif;

W_csOut = W_out - W_B;
#
# Mole transfer rate of solute to solid
#
Wm_solid = W_csIn - W_csOut;
****
FLOWSHEET

# Feeder

    Feed 1          is Input 1 of FEEDER
    Feed 2          is Input 2 of FEEDER
    Feed 3          is Input 3 of FEEDER
    Feed 4          is Input 4 of FEEDER
    Output 1 of FEEDER is Input 1 of IX1          Type LIQUID

# Column 1

    Output 1 of IX1    is Input 1 of IX2          Type LIQUID

# Column 2

    Output 1 of IX2    is Input 1 of IX3          Type LIQUID

# Column3

    Output 1 of IX3    is Input 1 of DECON_PRODUCT Type LIQUID

# Decontaminated Product

    Product 1          is Output 1 of DECON_PRODUCT

# CST Slurry Stream

    Connection 1 of CST_Info is Connection 1 of IX1
    Connection 2 of CST_info is Connection 1 of FEEDER
****
UNIT CST_Info IS a CST_Info
****
UNIT DECON_PRODUCT is a DECON_PRODUCT
Set
    nocomp = 51,
    liqcomp = 2,
    CsNO3 = 7,
    CsOH = 18,
    CsNO3b = 6,
    CsNO3a = 8,
    CsOHb = 17,
    CsOHa = 19
****
UNIT FEEDER is a FEEDER

```

```

Set
    nocomp = 51,
    liqcomp = 2,
    CsNO3 = 7,
    CsOH = 18
****
UNIT IX1 is an IX
    Set Nstage = 50
****
UNIT IX2 is an IX
    Set Nstage = 50
****
UNIT IX3 is an IX
    Set Nstage = 50
****
MACRO IX

    Model STAGE
    Model MONITOR

Flowsheet

# External Connections

    Feed    is Input  1 to STAGE 1          Type LIQUID

    Product is Output 1 of MONITOR          Type LIQUID

    Link     is Connection 1 of MONITOR

# Internal Connections

    ?Repeat
        Output 1 of STAGE ?(n) is
            Input 1 of STAGE ?(n+1)          Type LIQUID
    ?With n = < 1 : Nstage-1 >

    Output 1 of STAGE ?(Nstage) is Input 1 of MONITOR Type LIQUID
****
GLOBAL
    #=====#
    # Version Date: 29 September 1998 #
    #=====#
#
CONSTRAINTS
    FEEDER.out_molfrac(2)  = "IX1.Monitor".x_init;
    "IX1.Monitor".x_out(2) = "IX2.Monitor".x_init;
    "IX2.Monitor".x_out(2) = "IX3.Monitor".x_init;
    FEEDER.out_comp_conc(2) = "IX1.Monitor".c_init;
    "IX1.Monitor".out_comp_conc(2) = "IX2.Monitor".c_init;
    "IX2.Monitor".out_comp_conc(2) = "IX3.Monitor".c_init;

    ?Repeat
        "IX1.Stage(?(n)).rho_solvent = FEEDER.out_density;
        "IX1.Stage(?(n)).MW_solvent  = FEEDER.MW_solvent;

        "IX2.Stage(?(n)).rho_solvent = FEEDER.out_density;
        "IX2.Stage(?(n)).MW_solvent  = FEEDER.MW_solvent;

        "IX3.Stage(?(n)).rho_solvent = FEEDER.out_density;
        "IX3.Stage(?(n)).MW_solvent  = FEEDER.MW_solvent;
    ?With n = <1 : 50>

```

[illegible]

0. >

```

in4_flow      = 0.25.85# * (24/1500)      # kgal/day
in4_density   = 8.345                      # lb/gal
in4_massfrac  =
  < 1.        , 0.        , 0.        , 0.        , 0.        ,
    0.        , 0.        , 0.        , 0.        , 0.        ,
    0.        , 0.        , 0.        , 0.        , 0.        ,
    0.        , 0.        , 0.        , 0.        , 0.        ,
    0.        , 0.        , 0.        , 0.        , 0.        ,
    0.        , 0.        , 0.        , 0.        , 0.        ,
    0.        , 0.        , 0.        , 0.        , 0.        ,
    0.        , 0.        , 0.        , 0.        , 0.        ,
    0.        , 0.        , 0.        , 0.        , 0.        ,
  >

```

?Repeat

Within "IX1.STAGE(? (n))"

```

Stage_no      = ? (n)
NELEM         = 50                      # Number of axial elements
kf            = 0.23739 * 0.6          # m/hr
disp_coeff    = 0.79608 * 6E-3        # m2/hr
diff_coeff    = 5E-5 * 6E-3           # m2/hr
S             = .0730 * (5)'2         # m2, input D in ft.
deltaZ        = .3048*(16)/NELEM      # Length of axial element, m
epsilon       = 0.5                   # Void (Bulk)
eps_p         = 0.24                  # Void (Particle)
iso_A         = 2562/(1-epsilon)/(1-eps_p) # Iso const 1, L/L Solid
iso_B         = 33.26 * 132.9         # Iso const 2, L/mole Cs
diameter      = 3.75E-4              # Particle diameter, m

```

Within "IX2.STAGE(? (n))"

```

Stage_no      = ? (n)
NELEM         = 50                      # Number of axial elements
kf            = 0.23739 * 0.6          # m/hr
disp_coeff    = 0.79608 * 6E-3        # m2/hr
diff_coeff    = 5E-5 * 6E-3           # m2/hr
S             = .0730 * (5)'2         # m2, input D in ft.
deltaZ        = .3048*(16)/NELEM      # Length of axial element, m
epsilon       = 0.5                   # Void (Bulk)
eps_p         = 0.24                  # Void (Particle)
iso_A         = 2562/(1-epsilon)/(1-eps_p) # Iso const 1, L/L Solid
iso_B         = 33.26 * 132.9         # Iso const 2, L/mole Cs
diameter      = 3.75E-4              # Particle diameter, m

```

Within "IX3.STAGE(? (n))"

```

Stage_no      = ? (n)
NELEM         = 50                      # Number of axial elements
kf            = 0.23739 * 0.6          # m/hr
disp_coeff    = 0.79608 * 6E-3        # m2/hr
diff_coeff    = 5E-5 * 6E-3           # m2/hr
S             = .0730 * (5)'2         # m2, input D in ft.
deltaZ        = .3048*(16)/NELEM      # Length of axial element, m
epsilon       = 0.5                   # Void (Bulk)
eps_p         = 0.24                  # Void (Particle)
iso_A         = 2562/(1-epsilon)/(1-eps_p) # Iso const 1, L/L Solid
iso_B         = 33.26 * 132.9         # Iso const 2, L/mole Cs
diameter      = 3.75E-4              # Particle diameter, m

```

?With n = <1 : 50>

Within CST_Info

```

time          = t          # Process time, hr
column_diameter = 5.* 0.3048 # Column diameter, m
column_length = 16 * 0.3048 # Column length, m
CST_bulk_density = 62.43 * 0.13367 # CST bulk density, lb/gal

```

Initial

```

Within "IX1.Monitor"
  Cs_mass = 0.

```

```

Within "IX2.Monitor"
  Cs_mass = 0.

```

```

Within "IX3.Monitor"
  Cs_mass = 0.

```

```

?Repeat
  Within "IX1.STAGE(? (n))"
    c_A(1) = 0
    c_A(2) = 0
    c_A(3) = 0
    c_A_out = 0
  ?Repeat
    c_pA1(? (m)) = 0
    c_pA2(? (m)) = 0
    c_pA3(? (m)) = 0
    c_pA_out(? (m)) = 0
  ?With m = <1 : 4>

```

```

Within "IX2.STAGE(? (n))"
  c_A(1) = 0
  c_A(2) = 0
  c_A(3) = 0
  c_A_out = 0
?Repeat
  c_pA1(? (m)) = 0
  c_pA2(? (m)) = 0
  c_pA3(? (m)) = 0
  c_pA_out(? (m)) = 0
?With m = <1 : 4>

```

```

Within "IX3.STAGE(? (n))"
  c_A(1) = 0
  c_A(2) = 0
  c_A(3) = 0
  c_A_out = 0
?Repeat
  c_pA1(? (m)) = 0
  c_pA2(? (m)) = 0
  c_pA3(? (m)) = 0
  c_pA_out(? (m)) = 0
?With m = <1 : 4>
?With n = <1 : 50>

```

CONDITION

```

#If "IX1.MONITOR".DF >= 0.9 Then Stop
If "IX2.MONITOR".Cs_massconc >= 1.3E-6 Then Stop

```

REPORT OPERATION_100

Report Operation creates the Initial Subsection of OPERATION section

Number of axial elements: 100

\$ENDHELP

FIELDS

SCIENTIFIC

ZERO = 1e-12

NOBLANKS

DECIMALS = 6

&1 = "ix2.monitor".cs_mass;

&2 = "ix3.monitor".cs_mass;

?repeat

&?(2+20*(n-1)+1) = "ix2.stage(?n)".c_A(1);

&?(2+20*(n-1)+2) = "ix2.stage(?n)".c_A(2);

&?(2+20*(n-1)+3) = "ix2.stage(?n)".c_A(3);

&?(2+20*(n-1)+4) = "ix2.stage(?n)".c_A_out;

?repeat

&?(2+20*(n-1)+4+4*(m-1)+1) = "ix2.stage(?n)".c_pA1(?m);

&?(2+20*(n-1)+4+4*(m-1)+2) = "ix2.stage(?n)".c_pA2(?m);

&?(2+20*(n-1)+4+4*(m-1)+3) = "ix2.stage(?n)".c_pA3(?m);

&?(2+20*(n-1)+4+4*(m-1)+4) = "ix2.stage(?n)".c_pA_out(?m);

?With m = <1 : 4>

?With n = <1 : 100>

?repeat

&?(2002+20*(n-1)+1) = "ix3.stage(?n)".c_A(1);

&?(2002+20*(n-1)+2) = "ix3.stage(?n)".c_A(2);

&?(2002+20*(n-1)+3) = "ix3.stage(?n)".c_A(3);

&?(2002+20*(n-1)+4) = "ix3.stage(?n)".c_A_out;

?repeat

&?(2002+20*(n-1)+4+4*(m-1)+1) = "ix3.stage(?n)".c_pA1(?m);

&?(2002+20*(n-1)+4+4*(m-1)+2) = "ix3.stage(?n)".c_pA2(?m);

&?(2002+20*(n-1)+4+4*(m-1)+3) = "ix3.stage(?n)".c_pA3(?m);

&?(2002+20*(n-1)+4+4*(m-1)+4) = "ix3.stage(?n)".c_pA_out(?m);

?With m = <1 : 4>

?With n = <1 : 100>

FIELDMARK %

DISPLAY

OPERATION

Initial

Within "IX1.Monitor"

Cs_mass = %%%%%%%%%%

Within "IX2.Monitor"

Cs_mass = %%%%%%%%%%

Within "IX3.Monitor"

Cs_mass = 0.

?repeat

Within "IX1.STAGE(?n)"

c_A(1) = %%%%%%%%%%

c_A(2) = %%%%%%%%%%

c_A(3) = %%%%%%%%%%

c_A_out = %%%%%%%%%%

?repeat

c_pA1(?m) = %%%%%%%%%%

c_pA2(?m) = %%%%%%%%%%

c_pA3(?m) = %%%%%%%%%%

c_pA_out(?m) = %%%%%%%%%%

?With m = <1 : 4>

?With n = <1 : 100>

?repeat

Within "IX2.STAGE(?n)"

c_A(1) = %%%%%%%%%%


```

c_A(2) = %%%%%%%%%%%
c_A(3) = %%%%%%%%%%%
c_A_out = %%%%%%%%%%
?repeat
c_pA1(?m) = %%%%%%%%%%
c_pA2(?m) = %%%%%%%%%%
c_pA3(?m) = %%%%%%%%%%
c_pA_out(?m) = %%%%%%%%%%
?With m = <1 : 4>
?With n = <1 : 100>
?repeat
  Within "IX3.STAGE(?n)"
    c_A(1) = 0
    c_A(2) = 0
    c_A(3) = 0
    c_A_out = 0
    ?Repeat
      c_pA1(?m) = 0
      c_pA2(?m) = 0
      c_pA3(?m) = 0
      c_pA_out(?m) = 0
    ?With m = <1 : 4>
  ?With n = <1 : 100>

****
REPORT OPERATION_50
HELP
Report Operation creates the Initial Subsection of OPERATION section
Number of axial elements: 50
$ENDHELP
FIELDS
SCIENTIFIC
ZERO = 1e-12
NOBLANKS
DECIMALS = 6
&1 = "ix2.monitor".cs_mass;
&2 = "ix3.monitor".cs_mass;

?repeat
&?(2+20*(n-1)+1) = "ix2.stage(?n)".c_A(1);
&?(2+20*(n-1)+2) = "ix2.stage(?n)".c_A(2);
&?(2+20*(n-1)+3) = "ix2.stage(?n)".c_A(3);
&?(2+20*(n-1)+4) = "ix2.stage(?n)".c_A_out;
  ?repeat
&?(2+20*(n-1)+4+4*(m-1)+1) = "ix2.stage(?n)".c_pA1(?m);
&?(2+20*(n-1)+4+4*(m-1)+2) = "ix2.stage(?n)".c_pA2(?m);
&?(2+20*(n-1)+4+4*(m-1)+3) = "ix2.stage(?n)".c_pA3(?m);
&?(2+20*(n-1)+4+4*(m-1)+4) = "ix2.stage(?n)".c_pA_out(?m);
  ?With m = <1 : 4>
?With n = <1 : 50>

?repeat
&?(1002+20*(n-1)+1) = "ix3.stage(?n)".c_A(1);
&?(1002+20*(n-1)+2) = "ix3.stage(?n)".c_A(2);
&?(1002+20*(n-1)+3) = "ix3.stage(?n)".c_A(3);
&?(1002+20*(n-1)+4) = "ix3.stage(?n)".c_A_out;
  ?repeat
&?(1002+20*(n-1)+4+4*(m-1)+1) = "ix3.stage(?n)".c_pA1(?m);
&?(1002+20*(n-1)+4+4*(m-1)+2) = "ix3.stage(?n)".c_pA2(?m);
&?(1002+20*(n-1)+4+4*(m-1)+3) = "ix3.stage(?n)".c_pA3(?m);
&?(1002+20*(n-1)+4+4*(m-1)+4) = "ix3.stage(?n)".c_pA_out(?m);
  ?With m = <1 : 4>
?With n = <1 : 50>

```

FIELDMARK %
DISPLAY
OPERATION
Initial

```

Within "IX1.Monitor"
  Cs_mass = %%%%%%%%%%

Within "IX2.Monitor"
  Cs_mass = %%%%%%%%%%

Within "IX3.Monitor"
  Cs_mass = 0.
?repeat
  Within "IX1.STAGE(? (n))"
    c_A(1) = %%%%%%%%%%
    c_A(2) = %%%%%%%%%%
    c_A(3) = %%%%%%%%%%
    c_A_out = %%%%%%%%%%
    ?repeat
      c_pA1(? (m)) = %%%%%%%%%%
      c_pA2(? (m)) = %%%%%%%%%%
      c_pA3(? (m)) = %%%%%%%%%%
      c_pA_out(? (m)) = %%%%%%%%%%
    ?With m = <1 : 4>
  ?With n = <1 : 50>
?repeat
  Within "IX2.STAGE(? (n))"
    c_A(1) = %%%%%%%%%%
    c_A(2) = %%%%%%%%%%
    c_A(3) = %%%%%%%%%%
    c_A_out = %%%%%%%%%%
    ?repeat
      c_pA1(? (m)) = %%%%%%%%%%
      c_pA2(? (m)) = %%%%%%%%%%
      c_pA3(? (m)) = %%%%%%%%%%
      c_pA_out(? (m)) = %%%%%%%%%%
    ?With m = <1 : 4>
  ?With n = <1 : 50>
?repeat
  Within "IX3.STAGE(? (n))"
    c_A(1) = 0
    c_A(2) = 0
    c_A(3) = 0
    c_A_out = 0
    ?Repeat
      c_pA1(? (m)) = 0
      c_pA2(? (m)) = 0
      c_pA3(? (m)) = 0
      c_pA_out(? (m)) = 0
    ?With m = <1 : 4>
  ?With n = <1 : 50>

```

REPORT PROFILE
HELP

Generate the concentration profile in column 1
\$ENDHELP

FIELDS

scientific
zero = 1e-12
noblanks
decimals = 6

```
&1 = CST_Info.time * 60;
&2 = 1.0;
?Repeat
  &?(2+2*n-1) = ?(n)/50;
  &?(2+2*n) = "ix1.stage(?(n)).c_A_out/"ix1.stage(1)".c_A_in;
?With n = <1 : 50>
```

FIELDMARK %

DISPLAY

Concentration Profile in Column 1 at time = %%%%%%%%% minutes

```
Norm. Col. Length      Norm. Concentration
0.000000E-1           %%%%%%%%%
?Repeat
  %%%%%%%%%            %%%%%%%%%
?With n = <1 : 50>
```

REPORT SUMMARY

HELP

Summary of the cycle run results.

\$ENDHELP

SET

Case_name, Cycle_number

FIELDS

```
scientific
zero = 1e-10
noblanks
decimals = 5
&1 = Case_name;          # Case name
&2 = Cycle_number;       # Cycle number
&3 = CST_Info.cycle_time; # Cycle time
&4 = CST_Info.column_diameter/0.3048; # Column diameter, ft
&5 = CST_Info.column_length/0.3048;  # Column length, ft
&6 = feeder.inl_flow / 1.44;          # Feed stream flow rate (gpm)
&7 = feeder.inl_density;              # Feed stream density (lb/gal)
?Repeat
  &?(7+n) = feeder.inl_massfrac(?(n)); # Feed stream mass frxn
?With n = <1 : 51>
&59 = decon_product.out_flow/1.44; # Decon salt sol. flow rate (gpm)
&60 = decon_product.out_density;    # Decon salt sol. density (lb/gal)
?Repeat
  &?(60+n) = decon_product.out_massfrac(?(n)); # Decon salt sol. mass frxn
?With n = <1 : 51>
&112 = CST_Info.CST_mass;          # CST mass (lbs)
&113 = CST_Info.Cs_mass;           # Cs mass (lbs)
&114 = CST_Info.H2O_mass;          # Water mass (lbs)
&115 = 1000*CST_Info.Cs_mass/CST_Info.CST_mass; # Cs loading (mg Cs/g CST)
&116 = "ix1.stage(1)".in_comp_conc(2); # Cs conc along Col. 1
?Repeat
  &?(116+n) = "ix1.stage(?(5*n)).c_A_out;
?With n = <1 : 9>
&126 = "ix1.stage(50)".out_comp_conc(2);
&127 = "ix2.stage(1)".in_comp_conc(2); # Cs conc along Col. 2
?Repeat
  &?(127+n) = "ix2.stage(?(5*n)).c_A_out;
?With n = <1 : 9>
&137 = "ix2.stage(50)".out_comp_conc(2);
&138 = "ix3.stage(1)".in_comp_conc(2); # Cs conc along Col. 3
?Repeat
  &?(138+n) = "ix3.stage(?(5*n)).c_A_out;
```

```
?With n = <1 : 9>
&l48 = "ix3.stage(50)".out_comp_conc(2);
```

FIELDMARK %

DISPLAY

CASE: %%%%%%%%%%

Cycle Number: %%%%%%%%%%

Cycle Time (hrs): %%%%%%%%%%

Column Diameter (ft): %%%%%%%%%%

Column Length (ft): %%%%%%%%%%

Salt Feed Stream (Including Water and NaOH additions):

Flow rate (gpm): %%%%%%%%%%

Density (lb/gal): %%%%%%%%%%

Mass fraction: %%%%%%%%%%

1. H2O
2. Misc. salts
3. NaNO3
4. NaNO2
5. NaOH
6. KNO3
7. CsNO3
8. NH4NO3
9. NH4OH
10. NaAlO2
11. Misc. sludge
12. Na2U2O7
13. Fe(OH)3
14. Al(OH)3
15. Cr(OH)2
16. C6H6
17. Phenol/Phenoxide
18. CsOH
19. KOH
20. CsB(C6H5)4
21. NaB(C6H5)4
22. Na2(C6H5)BO2
23. KB(C6H5)4
24. NH4B(C6H5)4
25. NaTi2O5H
26. NaT.S(OH)2
27. NaT.Na2U2O7
28. (C6H5)3B
29. (C6H5)2BOH
30. (C6H5)B(OH)2
31. B(OH)3
32. K2O
33. LiO2
34. MO
35. MnO
36. TiO2
37. U3O8
38. ZrO2
39. Ca3P2O8
40. P2O5
41. Cr2O3
42. CsO2
43. CuO
44. Na2O

45. NiO
46. SiO₂
47. HgO
48. alpha (PuO₂)
49. CaCO₃
50. Na₂CO₃
51. Na₂SO₄

Water to load CST (gals):
2M NaOH solution (gals):
Excess water to unload CST (gals):

47100.
23500.
25950.

```
Flow rate (gpm):      %%%%%%%%%%%
Density (lb/gal):    %%%%%%%%%%%
Mass fraction:       %%%%%%%%%%%
```

1. H₂O
2. Misc. salts
3. NaNO₃
4. NaNO₂
5. NaOH
6. KNO₃
7. CsNO₃
8. NH₄NO₃
9. NH₄OH
10. NaAlO₂
11. Misc. sludge
12. Na₂U₂O₇
13. Fe(OH)₃
14. Al(OH)₃
15. Cr(OH)₂
16. C₆H₆
17. Phenol/Phenoxide
18. CsOH
19. KOH
20. CsB(C₆H₅)₄
21. NaB(C₆H₅)₄
22. Na₂(C₆H₅)BO₂
23. KB(C₆H₅)₄
24. NH₄B(C₆H₅)₄
25. NaTi₂O₅H
26. NaT.S(OH)₂
27. NaT.Na₂U₂O₇
28. (C₆H₅)₃B
29. (C₆H₅)₂BOH
30. (C₆H₅)B(OH)₂
31. B(OH)₃
32. K₂O
33. Li₂O
34. MO
35. MnO
36. TiO₂
37. U₃O₈
38. ZrO₂
39. Ca₃P₂O₈
40. P₂O₅
41. Cr₂O₃
42. CsO₂
43. CuO
44. Na₂O
45. NiO
46. SiO₂

[illegible]

47. HgO
48. alpha (PuO2)
49. CaCO3
50. Na2CO3
51. Na2SO4

```
Solid CST (lbs):      %%%%%%%%%%
Cs (lbs):             %%%%%%%%%%
Water (lbs):          %%%%%%%%%%
```

Cs Concentration (mol/L) in the Salt Solution along Column 1
(Values given at equal distance between inlet and outlet)

[illegible][illegible]

Outlet: %%%%%%%%%%

[illegible]

Outlet: %%%%%%%%%%

* * * *

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