APPENDIX FIVE

THE PROGRAM CODE FOR THE COSAN MODEL

The method outlined fixes certain values of **V**, the matrix of orthogonal variates, to be zero, depending on how many canonical variates are to be modeled. Those variates to be estimated in the model are unrestricted. The columns of **V** not modeled are dummy variates for the purpose of making **V** orthogonal. Suppose there are *t* of these dummy variates. If $t = 1$, then the first *p*-1 columns of **V** determine the p^{th} column and it is not necessary to fix any elements of **V** to be zero. If $t = 2$, then the first *p*-2 columns are unrestricted. Set an arbitrary element of the $(p-1)^{th}$ vector to be zero to fix it, and the and the p^{th} vector follows. If $t = 3$, then set two elements of the $(p-2)^{th}$ column to be zero, and one element of the $(p-1)^{th}$ vector. One continues in this manner to constrain the desired number of variates.

Now in the COSAN model these elements of **V** cannot be directly set equal to zero because **V** is not directly estimated. Instead, **H** is directly estimated, where **V** is a function of **H**, $\mathbf{V} = (\mathbf{I} - \mathbf{H}')^{-1}(\mathbf{I} - \mathbf{H})$. However, since specific elements of **H** do not correspond to specific elements of **V**, the restrictions must be put on $(\mathbf{I} - \mathbf{H}')^{-1}(\mathbf{I} - \mathbf{H})$ indirectly. This is done by pre-multiplying and post-multiplying $(\mathbf{I} - \mathbf{H}')^{-1}(\mathbf{I} - \mathbf{H})$ by specific matrices to select for the appropriate elements. These are then set equal to zero by placing zeros in the data matrix.

Pre-multiply **V** $(= (\mathbf{I}_{(p)} + \mathbf{H})^{-1}(\mathbf{I}_{(p)} - \mathbf{H}))$ by a diagonal matrix with ones on the last *t*-1 diagonal elements and call this matrix **J**. Post-multiply **V** by a matrix with a 1 on the t^{th} diagonal element, and zeros elsewhere and call this matrix **K**. This yields a matrix with zeros in all columns except the t^{th} column, which has the last *t*-1 elements of the t^{th} column of **V**. Call this **U**. Then in the COSAN model set $\mathbf{UU}'$ equal to a $p \times p$ matrix of zeros.

For example, to set three elements of the $(p-3)^{th}$ column of **V** to zero, choose **J** and **K** such that $\mathbf{U} = \mathbf{JVK}$, where:

$$\mathbf{U}=\begin{bmatrix} 0 & & & & & & \\ & \ddots & & & & & \\ & & 0 & & & & \\ & & & 0 & & & \\ & & & & 1 & & \\ & & & & & 1 & \\ & & & & & & 1 \end{bmatrix}\mathbf{V}\begin{bmatrix} 0 & & & & & & \\ & \ddots & & & & & \\ & & 0 & & & & \\ & & & 1 & & & \\ & & & & 0 & & \\ & & & & & 0 & \\ & & & & & & 0 \end{bmatrix}=\begin{bmatrix} 0 & & & & & & \\ & \ddots & & & & & \\ & & 0 & & & & \\ & & & 0 & 0 & 0 & 0 \\ & & & v_{p-4,p-3} & 0 & 0 & 0 \\ & & & v_{p-5,p-3} & 0 & 0 & 0 \\ & & & v_{p-6,p-3} & 0 & 0 & 0 \end{bmatrix}$$

Now in the COSAN model one places $\mathbf{UU}' = \mathbf{Z}$, where $\mathbf{Z}$ is a $p \times p$ matrix of zeros. Thus one has set the three elements of $\mathbf{V}$ to zero, $v_{p-4,p-3}$, $v_{p-5,p-3}$ and $v_{p-6,p-3}$. Such a statement must be set up for each dummy variate in the model except the first.

To the data matrix, that is, the between groups covariance matrix $\mathbf{S}$, append p rows and p columns of zeros, so

$$\mathbf{S}^* = \begin{bmatrix} \mathbf{S} & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}.$$

In the code note the following. The fit function is least squares. There are 42 variables, 28 for the streamwater variables, 14 for the dummy variables. The first line of the COSAN statement is

```
t(42,gen,inv)*v(42,gen)*r(42,sym)*p1(42,sym).
```

The block diagonal matrices for $\mathbf{V}$ are `t(42,gen,inv)*v(42,gen)`. `r(42,sym)` is a matrix whose diagonal elements have the root variances explained. The next lines in the COSAN statement, starting with

```
s1a(42,sym)*ta(42,gen,inv)*va(42,gen)*s1b(42,sym)
```

restrict the selected elements of $\mathbf{V}$ to be zero as described earlier; `Ta(42,gen,inv)*va(42,gen)` is a matrix with $\mathbf{V}$ in its bottom block diagonal; `S1a(42,sym)` and `s1b(42,sym)` correspond to the matrices $\mathbf{J}$ and $\mathbf{K}$ from above.

The full code follows below.

```
libname shen 'c:\prg\shen';
proc calis cov data=shen.z11 method=U outest=cal
omethod=cg maxiter=1000 maxfunc=2000 nostderr privec; title ' ';


*The variables statement defines the variables.  Variables with an "a" as a
 suffix indicate the first occasion, those a "b" indicate the second
 occasion, and those with a "z" indicate the the dummies which are set to
 zero.;



var dischа conda pha tempa caa mga naa ka alka so4a c1a sia no3a nh4a
    dischb condb phb tempb cab mgb nab kb alkb so4b c1b sib no3b nh4b
    dischz condz phz tempz caz mgz naz kz alkz so4z c1z siz no3z nh4z;
```

```
*The "cosan" statement defines the model.  t, v, r and p are matrices.  In
 the model the inverse of t is modeled.;

cosan t(42,gen,inv)*v(42,gen)*r(42,sym)*p1(42,sym)+
      s1a(42,sym)*ta(42,gen,inv)*va(42,gen)*s1b(42,sym)+
      s2a(42,sym)*ta(42,gen,inv)*va(42,gen)*s2b(42,sym)+
      s3a(42,sym)*ta(42,gen,inv)*va(42,gen)*s3b(42,sym)+
      s4a(42,sym)*ta(42,gen,inv)*va(42,gen)*s4b(42,sym)+
      s5a(42,sym)*ta(42,gen,inv)*va(42,gen)*s5b(42,sym)+
      s6a(42,sym)*ta(42,gen,inv)*va(42,gen)*s6b(42,sym)+
      s7a(42,sym)*ta(42,gen,inv)*va(42,gen)*s7b(42,sym)+
      s8a(42,sym)*ta(42,gen,inv)*va(42,gen)*s8b(42,sym)+
      s9a(42,sym)*ta(42,gen,inv)*va(42,gen)*s9b(42,sym)+
      s10a(42,sym)*ta(42,gen,inv)*va(42,gen)*s10b(42,sym)+
      s11a(42,sym)*ta(42,gen,inv)*va(42,gen)*s11b(42,sym)+
      s12a(42,sym)*ta(42,gen,inv)*va(42,gen)*s12b(42,sym);


*The "matrix" statement sets the matrix elements equal to parameters or
 constants.  "{1,2}=v12"  sets the element in the first row and second
 column equal to the parameter v12.  Matrix elements not specified default
 to zero values.;

matrix t
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 {15,15}=-1,{16,16}=-1,{17,17}=-1,{18,18}=-1,{19,19}=-1,{20,20}=-1,{21,21}=-1,
 {22,22}=-1,{23,23}=-1,{24,24}=-1,{25,25}=-1,{26,26}=-1,{27,27}=-1,{28,28}=-1,
 {29,29}=1,{30,30}=1,{31,31}=1,{32,32}=1,{33,33}=1,{34,34}=1,{35,35}=1,
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{24,25}=t82,{24,26}=t83,{24,27}=t84,{24,28}=t85,
{25,26}=t86,{25,27}=t87,{25,28}=t88,{26,27}=t89,{26,28}=t90,{27,28}=t91;

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{1,15}=1, {2,16}=1, {3,17}=1, {4,18}=1, {5,19}=1, {6,20}=1, {7,21}=1,{8,22}=1,
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{1,29}=1, {2,30}=1, {3,31}=1, {4,32}=1, {5,33}=1, {6,34}=1, {7,35}=1,{8,36}=1,
{9,37}=1,{10,38}=1,{11,39}=1,{12,40}=1,{13,41}=1,{14,42}=1,


{15,1}=1, {16,2}=1, {17,3}=1, {18,4}=1, {19,5}=1, {20,6}=1, {21,7}=1,{22,8}=1,
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{15,15}=1, {16,16}=1, {17,17}=1, {18,18}=1, {19,19}=1, {20,20}=1, {21,21}=1,
{22,22}=1,{23,23}=1,{24,24}=1,{25,25}=1,{26,26}=1,{27,27}=1,{28,28}=1,

{15,29}=1, {16,30}=1, {17,31}=1, {18,32}=1, {19,33}=1, {20,34}=1, {21,35}=1,
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{29,1}=1, {30,2}=1, {31,3}=1, {32,4}=1, {33,5}=1, {34,6}=1, {35,7}=1,{36,8}=1,
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{29,15}=1, {30,16}=1, {31,17}=1, {32,18}=1, {33,19}=1, {34,20}=1, {35,21}=1,
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{36,36}=1,{37,37}=1,{38,38}=1,{39,39}=1,{40,40}=1,{41,41}=1,{42,42}=1;

matrix r
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{8,8}=d1d8,{9,9}=d1d9,{10,10}=d1d10,

{15,15}=d2d1,{16,16}=d2d2,{17,17}=d2d3,{18,18}=d2d4,{19,19}=d2d5,
{20,20}=d2d6,{21,21}=d2d7,{22,22}=d2d8,{23,23}=d2d9,{24,24}=d2d10;

matrix ta
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{29,37}=v8,{29,38}=v9,{29,39}=v10,{29,40}=v11,{29,41}=v12,{29,42}=v13,
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{39,40}=v86,{39,41}=v87,{39,42}=v88,{40,41}=v89,{40,42}=v90,{41,42}=v91,

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{39,38}=t82,{40,38}=t83,{41,38}=t84,{42,38}=t85,
{40,39}=t86,{41,39}=t87,{42,39}=t88,{41,40}=t89,{42,40}=t90,{42,41}=t91;

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 {22,22}=1,{23,23}=1,{24,24}=1,{25,25}=1,{26,26}=1,{27,27}=1,{28,28}=1,

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{36,29}=v7,
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{39,38}=v82,{40,38}=v83,{41,38}=v84,{42,38}=v85,
{40,39}=v86,{41,39}=v87,{42,39}=v88,{41,40}=v89,{42,40}=v90,{42,41}=v91,

{29,30}=t1,{29,31}=t2,{29,32}=t3,{29,33}=t4,{29,34}=t5,{29,35}=t6,{29,36}=t7,
{29,37}=t8,{29,38}=t9,{29,39}=t10,{29,40}=t11,{29,41}=t12,{29,42}=t13,
{30,31}=t14,{30,32}=t15,{30,33}=t16,{30,34}=t17,{30,35}=t18,{30,36}=t19,
```

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{38,39}=t82,{38,40}=t83,{38,41}=t84,{38,42}=t85,
{39,40}=t86,{39,41}=t87,{39,42}=t88,{40,41}=t89,{40,42}=t90,{41,42}=t91;



matrix s1a
{42,42}=1;
matrix s1b
{41,41}=1;
matrix s2a
{42,42}=1, {41,41}=1;
matrix s2b
{40,40}=1;
matrix s3a
{42,42}=1,{41,41}=1,{40,40}=1;
matrix s3b
{39,39}=1;
matrix s4a
{42,42}=1,{41,41}=1,{40,40}=1,{39,39}=1;
matrix s4b
{38,38}=1;
matrix s5a
{42,42}=1,{41,41}=1,{40,40}=1,{39,39}=1,{38,38}=1;
matrix s5b
{37,37}=1;
matrix s6a
{42,42}=1,{41,41}=1,{40,40}=1,{39,39}=1,{38,38}=1,{37,37}=1;
matrix s6b
{36,36}=1;
matrix s7a
{42,42}=1,{41,41}=1,{40,40}=1,{39,39}=1,{38,38}=1,{37,37}=1,{36,36}=1;
matrix s7b
{35,35}=1;
matrix s8a
{42,42}=1,{41,41}=1,{40,40}=1,{39,39}=1,{38,38}=1,{37,37}=1,{36,36}=1,
{35,35}=1;
matrix s8b
{34,34}=1;
matrix s9a
{42,42}=1,{41,41}=1,{40,40}=1,{39,39}=1,{38,38}=1,{37,37}=1,{36,36}=1,
{35,35}=1,{34,34}=1;
matrix s9b
{33,33}=1;
matrix s10a
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{35,35}=1,{34,34}=1,{33,33}=1;
matrix s10b
{32,32}=1;
```

```
matrix s11a
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{35,35}=1,{34,34}=1,{33,33}=1,{32,32}=1;
matrix s11b
{31,31}=1;
matrix s12a
{42,42}=1,{41,41}=1,{40,40}=1,{39,39}=1,{38,38}=1,{37,37}=1,{36,36}=1,
{35,35}=1,{34,34}=1,{33,33}=1,{32,32}=1,{31,31}=1;
matrix s12b
{30,30}=1;


*What follows are SAS programming statements that constrain the
 parameters.  t1=-v1 constrains t1 to be the additive inverse of v1.;

t1=-v1;t2=-v2;t3=-v3;t4=-v4;t5=-v5;t6=-v6;t7=-v7;t8=-v8;t9=-v9;t10=-v10;
t11=-v11;t12=-v12;t13=-v13;t14=-v14;t15=-v15;t16=-v16;t17=-v17;t18=-v18;
t19=-v19;t20=-v20;t21=-v21;t22=-v22;t23=-v23;t24=-v24;t25=-v25;t26=-v26;
t27=-v27;t28=-v28;t29=-v29;t30=-v30;t31=-v31;t32=-v32;t33=-v33;t34=-v34;
t35=-v35;t36=-v36;t37=-v37;t38=-v38;t39=-v39;t40=-v40;t41=-v41;t42=-v42;
t43=-v43;t44=-v44;t45=-v45;t46=-v46;t47=-v47;t48=-v48;t49=-v49;t50=-v50;
t51=-v51;t52=-v52;t53=-v53;t54=-v54;t55=-v55;t56=-v56;t57=-v57;t58=-v58;
t59=-v59;t60=-v60;t61=-v60;t62=-v62;t63=-v63;t64=-v64;t65=-v65;t66=-v66;
t67=-v67;t68=-v68;t69=-v69;t70=-v70;t71=-v71;t72=-v72;t73=-v73;t74=-v74;
t75=-v75;t76=-v76;t77=-v77;t78=-v78;t79=-v79;t80=-v80;t81=-v81;t82=-v82;
t83=-v83;t84=-v84;t85=-v85;t86=-v86;t87=-v87;t88=-v88;t89=-v89;t90=-v90;
t91=-v91;


d1d2=0;d1d3=0;d1d4=0;d1d5=0;d1d6=0;d1d7=0;d1d8=0;d1d9=0;d1d10=0;
d2d2=0;d2d3=0;d2d4=0;d2d5=0;d2d6=0;d2d7=0;d2d8=0;d2d9=0;d2d10=0;

run;



*The subsequent code calculates V.;

 proc iml; use cal; read point 4
 var {v1 v2 v3 v4 v5 v6 v7 v8 v9 v10 v11 v12 v13 v14 v15
 v16 v17 v18 v19 v20 v21 v22 v23 v24 v25 v26 v27 v28 v29 v30 v31 v32 v33 v34
 v35 v36 v37 v38 v39 v40
 v41 v42 v43 v44 v45 v46 v47 v48 v49 v50 v51 v52 v53 v54 v55 v56 v57 v58 v59
 v60 v61 v62 v63 v64 v65
 v66 v67 v68 v69 v70 v71 v72 v73 v74 v75 v76 v77 v78 v79 v80 v81 v82 v83 v84
 v85 v86 v87 v88 v89 v90 v91} into K;




 v=J(14,14,0);
 v[1,2]=K[,1]; v[1,3]=K[,2]; v[1,4]=K[,3];    v[1,5]=K[,4];  v[1,6]=K[,5];
 v[1,7]=K[6]; v[1,8]=K[7];
 v[1,9]=K[,8]; v[1,10]=K[,9];v[1,11]=K[,10];  v[1,12]=K[,11];v[1,13]=K[,12];
 v[1,14]=K[,13];
 v[2,3]=K[,14]; v[2,4]=K[,15]; v[2,5]=K[,16]; v[2,6]=K[,17]; v[2,7]=K[,18];
 v[2,8]=K[,19];v[2,9]=K[,20];
 v[2,10]=K[,21];v[2,11]=K[,22];v[2,12]=K[,23];v[2,13]=K[,24];v[2,14]=K[,25];
 v[3,4]=K[,26]; v[3,5]=K[,27]; v[3,6]=K[,28]; v[3,7]=K[,29]; v[3,8]=K[,30];
```

```
v[3,9]=K[,31];
v[3,10]=K[,32];v[3,11]=K[,33];v[3,12]=K[,34];v[3,13]=K[,35];v[3,14]=K[,36];
v[4,5]=K[,37]; v[4,6]=K[,38]; v[4,7]=K[,39]; v[4,8]=K[,40]; v[4,9]=K[,41];
v[4,10]=K[,42];v[4,11]=K[,43];v[4,12]=K[,44];v[4,13]=K[,45];v[4,14]=K[,46];
v[5,6]=K[,47]; v[5,7]=K[,48]; v[5,8]=K[,49]; v[5,9]=K[,50];
v[5,10]=K[,51];v[5,11]=K[,52];v[5,12]=K[,53];v[5,13]=K[,54];v[5,14]=K[,55];
v[6,7]=K[,56]; v[6,8]=K[,57]; v[6,9]=K[,58];
v[6,10]=K[,59];v[6,11]=K[,60];v[6,12]=K[,61];v[6,13]=K[,62];v[6,14]=K[,63];
v[7,8]=K[,64]; v[7,9]=K[,65]; v[7,10]=K[,66];v[7,11]=K[,67];v[7,12]=K[,68];
v[7,13]=K[,69];v[7,14]=K[,70];
v[8,9]=K[,71]; v[8,10]=K[,72];v[8,11]=K[,73];v[8,12]=K[,74];v[8,13]=K[,75];
v[8,14]=K[,76];
v[9,10]=K[,77];v[9,11]=K[,78];v[9,12]=K[,79];v[9,13]=K[,80];v[9,14]=K[,81];
v[10,11]=K[,82];v[10,12]=K[,83];v[10,13]=K[,84];v[10,14]=K[,85];
v[11,12]=K[,86];v[11,13]=K[,87];v[11,14]=K[,88];v[12,13]=K[,89];
v[12,14]=K[,90];v[13,14]=K[,91];
Vo=v-v`-I(14); To=-v+v`-I(14);
Orth=inv(Vo)*To; print orth;
```

*The matrix of canonical variates, **V**, is called “orth”.;