Appendix A

SAS code used in determining the calibrated parameter estimates for the SAPS net alkalinity generation model. Code follows input data. Developed by Bob Noble

```
%macro mixer(y=,x=,numvar=,w=);

  %let nva = &w;
  %let nwv = %eval(1000-&w);

  %let datset = %str(va wv);
  %do i = 1 %to 2;

    %let t = %scan(&datset,&i,' ');

    proc means data=&t noprint;
      var &y &x;
      output out=avg mean=&y &x;
    run;

    proc means data=&t noprint;
      var &y &x;
      output out=stdev std=&y &x;
    run;

    proc standard data=&t mean=0 std=1 out=dat;
      var &y &x;
    run;

    data z1;
      do i = 1 to &&n&t;
        %do j = 1 %to &numvar;
```

```
z&j = rannor(0);
      %end;

      output;
    end;
  run;

  proc princomp data=z1 noprint out=z2;
    var %do j = 1 %to &numvar; z&j %end;;
  run;

  proc standard data=z2 mean=0 std=1 out=z3;
    var  %do j = 1 %to &numvar; prin&j %end;;
  run;

  proc iml;
    use z3;
    read all var { %do j = 1 %to &numvar; prin&j %end; } into d;
    use dat;
    read all var {&y &x} into corr;
    r = corr` * corr # (1/(nrow(corr)-1));
    z = d*eigvec(r)*diag(sqrt(eigval(r)))*eigvec(r)`;
    create corr var {&y &x};
    append from z;

  proc standard data=corr mean=0 std=1 out=corr2;
    var &y &x;
  run;

  proc iml;
    use avg;
    read all var {&y &x} into avg;
    use stdev;
    read all var {&y &x} into stdev;
    use corr2;
    read all var {&y &x} into z;
    x = j(nrow(z),ncol(z),.);
    do i = 1 to nrow(z);
      do j = 1 to ncol(z);
        x[i,j] = avg[1,j]+stdev[1,j]*z[i,j];
      end;
    end;
    create fin&t var {y &x};
    append from x;

%end;

data tot;
  set finva finwv;
run;
```

```
  proc iml;
    use tot;
    read all var {&x} into x;
    read all var {&y} into y;
    n = nrow(y);
    u = j(n,1,1);
    x = u||x;
    print "Model:&nva, Calibration:&nwv";
    b = inv(x`*x)*x`*y;
    mattrib b rowname={INTERCEP &x} label='';
    print b;
    sse = (y-x*b)`*(y-x*b);
    g = inv(u`*u)*u`*y;
    sst = (y-u*g)`*(y-u*g);
    rsq = 1 - sse/sst;
    mattrib rsq rowname={'R-square'} label='';
    print rsq;
%mend;

/*-----------------------------------------------------------+
 |                                                           |
 |  y = response variable                                    |
 |  x = string of independent variables for the model        |
 |  numvar = number of independent variables in model + 1    |
 |  w = weight of model data. w is an integer, 1<w<999       |
 |                                                           |
 +-----------------------------------------------------------*/
%mixer(y=%str(y),
       x=%str(lntr  fe  mnacid ),
       numvar=4,
       w=100);

quit;
```