CAP88-PC V4 TRAINING

Module 2.2

Models, Methods, File Structures

Major Changes Visible to User

Age Dependent Dose and Risk Factors from ORNL DCFPAK 2.2

- Ingestion
- Inhalation

Updated User Interface

- File Management (Migration and Data Locations)
- Report Generation
- Look and Feel (Windows standard but retain earlier screen style)

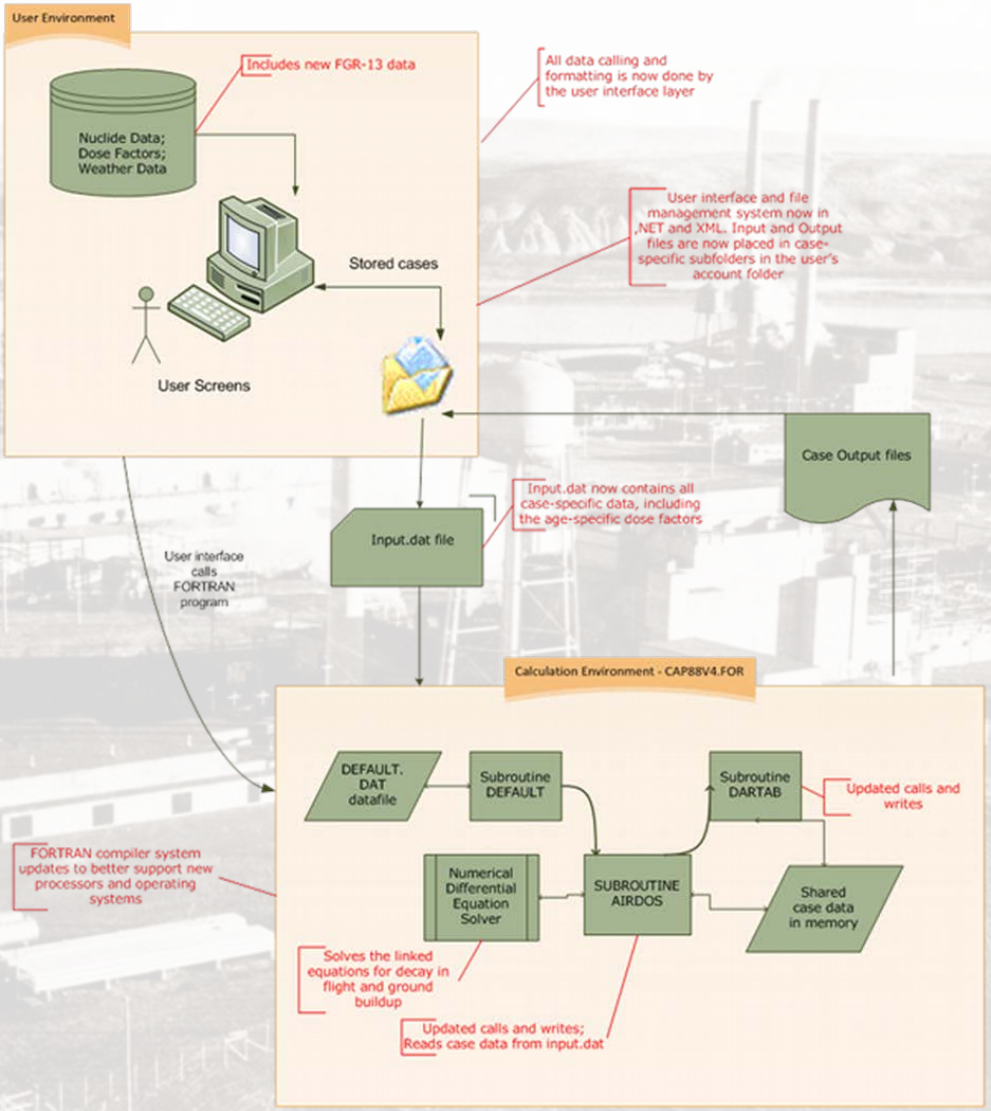
Radionuclide Set

- 1252 Total Radionuclides (737 with internal DCFs)
- Flags Radionuclides with External but not Internal DCF
- Up to 500 isotopes in a run

Major Architecture Changes

- Separation of data from calcs
- New data relationships
- Single FORTRAN code
- No temp files
- Standard variable naming
- Updated data and code standards

SPEED
MAINTAINABILITY



Model Changes

First: What Hasn't Changed?

Long-term Gaussian Plume Air Dispersion Model

Regulatory Guide 1.109 Food Chain Accumulation Model

Format for Wind and Population Files
- some minor changes
- general functionality unchanged

EPA Mandated Values for Certain Model Variables, e.g.
- deposition velocity
- scavenging coefficient

Radon-Only Case Model

Major Model Changes

Age-Dependent DCFPAK 2.2 Values for Dose and Risk Factors

- Build dose/risk factors in user interface code
- 26 dose organs incl. Whole Body (still 15 risk organs)

Age Dependent Inhalation and Ingestion Rates

- Values compiled by EPA from 2009 Exposure Factors Handbook

Implementation of Numerical Solver for Chain Decay and Deposition

- Handles chains up to 30 isotopes deep + branching
- Chains defined in DCFPAK data, translated to XML
- Implemented at each sector for air and ground surface
- Replaces approximate methods used in V3
- DLSODE solver package

New Compilers Allow Full Double Precision and Partial Vectorization

- reducing run time and eliminating underflow crashes were priorities

Some Other Changes

Enhanced Installation and Run Logging

All Case Information in One Location

- Report Generation – Output Files Stored in Dataset Folder
- Input Pop and Wnd Files in Dataset Folder

Greatly Increased Source Ranges (1E-25 to 1E+28 Ci/yr)

Increased Input Validation, Viewable in Errors Window

Edits Displayed in Real Time in the Changes Window

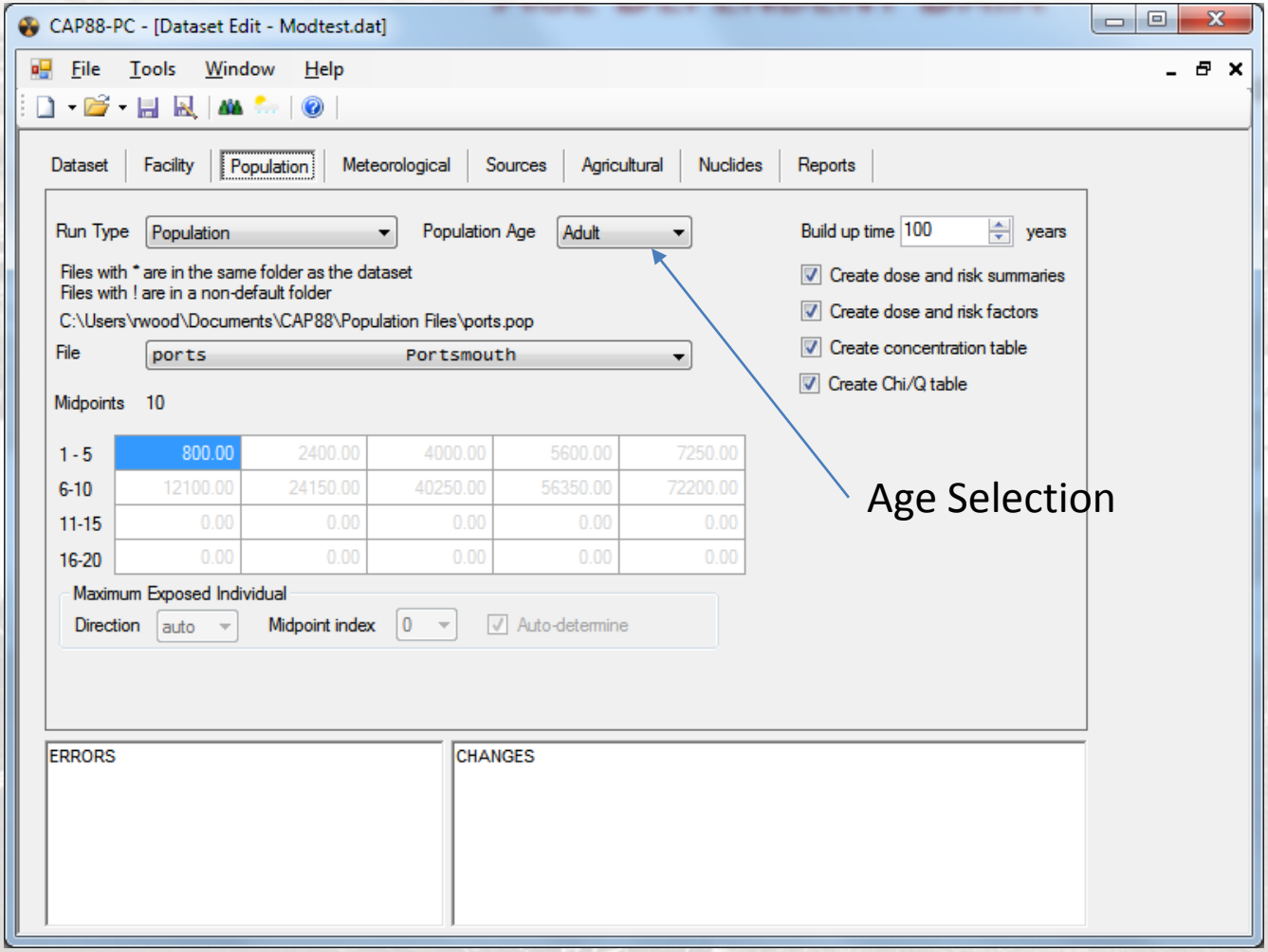
Elimination of Supporting MS Access Databases

Expanded On-Line Help System

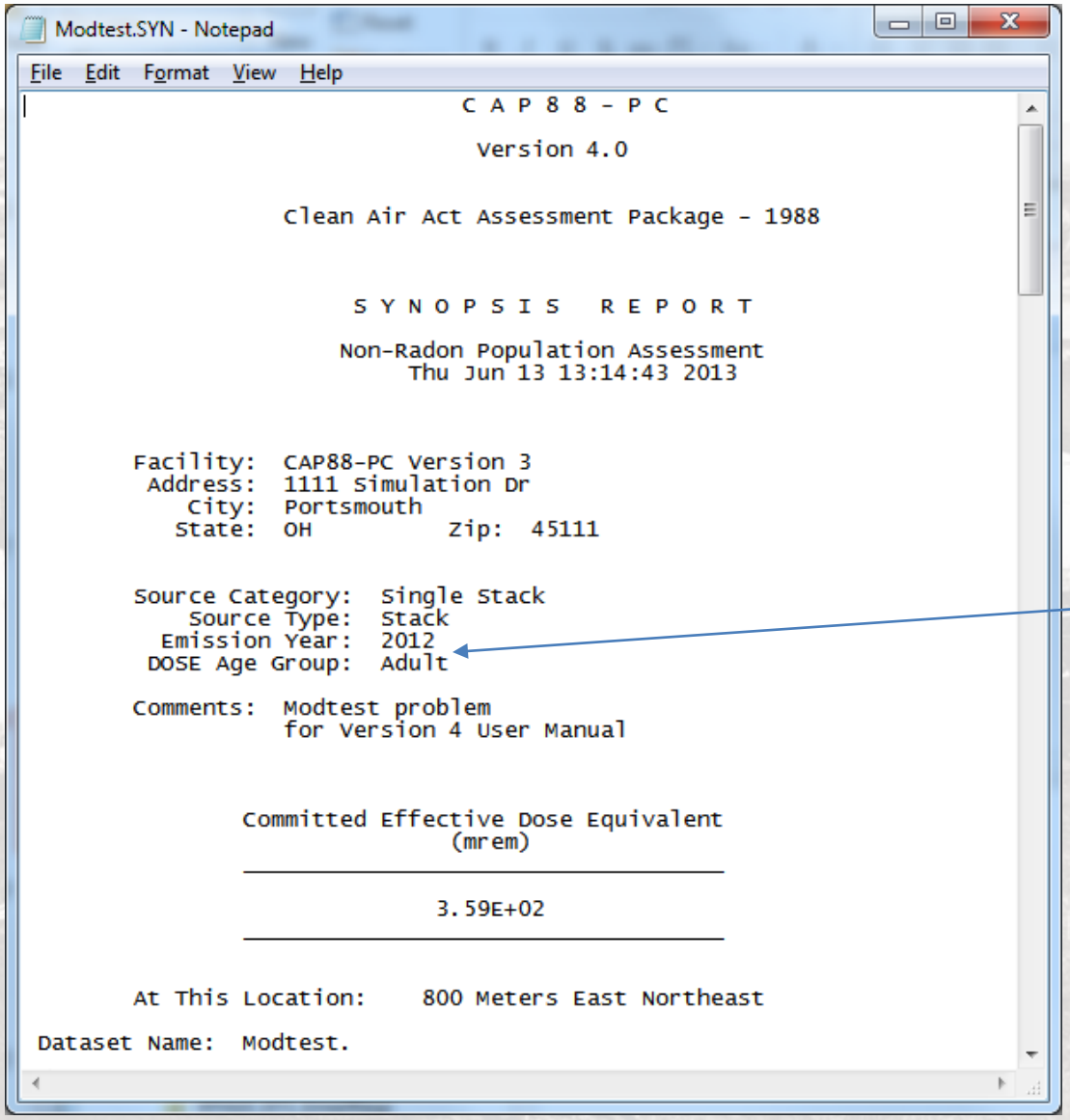
Digital Code Signature to Support Code Security Requirements

Age Dependent Data

Six age groups: 100 day old, 1 year old, 5 year old, 10 year old, 15 year old, Adult



Age Data Reporting



Printed In Synopsis, Summary, and Factors files. (.syn, .sum, .fac)

Age Data Implementation

All dose calculations for that dataset use the age-selected factors
- Max individual dose is for that age
- Population is assumed to all be at that age

Ingestion and Inhalation data are for the selected age group
- Individual intake rates
- All population intake rates

Why this approach:
- Programming implementation
- Uncertainty in direction of regulation (written with adult factors in mind)
- Other approaches for population would have imposed major compliance burden
  - New population data with age dependency

Future possible approaches:
- Loop all age groups and select highest dose result
- Require age-dependent receptor data
- Make assumptions on age distributions within the receptor population

This first use is only a step, full implementation will require policy changes

New Ground Surface Buildup model

Need to calculate ground surface activity for all isotopes at a given time
- Additive terms are deposition and radioactive ingrowth
-removal terms are leaching and radioactive decay

$$\frac{dn_1}{dt} = R_1 - \lambda_1^{e} n_1(t), \text{where } \lambda_1^{e} \equiv \lambda_1 + \lambda_{l,1} \text{ for first member of chain}$$

R term is production term, includes sum of all decay chain contributors for progeny

Version 2 used pre-defined factors for a limited number of chains
Version 3 used approximate method performed in Visual Basic front end
Both methods had weaknesses

Ground Surface Matrix Representation

$$\begin{bmatrix} dn_1/dt \\ dn_2/dt \\ dn_3/dt \\ \vdots \\ dn_i/dt \\ \vdots \\ dn_{N-1}/dt \\ dn_N/dt \end{bmatrix} = \begin{bmatrix} R_1 \\ R_2 \\ R_3 \\ \vdots \\ R_i \\ \vdots \\ R_{N-1} \\ R_N \end{bmatrix} + \begin{bmatrix} -\lambda_1^e & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 \\ \lambda_{12} & -\lambda_2^e & 0 & \cdots & 0 & \cdots & 0 & 0 \\ \lambda_{13} & \lambda_{23} & -\lambda_3^e & \cdots & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & & \vdots & \vdots \\ \lambda_{1i} & \lambda_{2i} & \lambda_{3i} & \cdots & -\lambda_i^e & & 0 & 0 \\ \vdots & \vdots & \vdots & & & \ddots & \vdots & \vdots \\ \lambda_{1,N-1} & \lambda_{2,N-1} & \lambda_{3,N-1} & \cdots & \lambda_{N-1,j} & \cdots & -\lambda_{N-1}^e & 0 \\ \lambda_{1,N} & \lambda_{2,N} & \lambda_{3,N} & \cdots & \lambda_{N,j} & \cdots & \lambda_{N,N-1} & -\lambda_N^e \end{bmatrix} \begin{bmatrix} n_1(t) \\ n_2(t) \\ n_3(t) \\ \vdots \\ n_i(t) \\ \vdots \\ n_{N-1}(t) \\ n_N(t) \end{bmatrix}$$

Note that lambda values must include branching fractions

GROUND CONCENTRATION FORMULATION IN FORTRAN

```
      SUBROUTINE f_gc(n,t,yg,ydotg)

      IMPLICIT NONE

<<<<<<< .mine
      INTEGER n, i
      DOUBLE PRECISION t_end,y(30)
=======
      INTEGER n, i, j
      DOUBLE PRECISION t,yg(*),lame(30),blam(30,30),deptot(30)
      Double Precision first(30), ydotg(*), lam(30), atchi(30)
      Common /gcfuncdat/ lame,blam,deptot
>>>>>>> .r203

       Do 5 i=1,30
          first(i)=0.d0
     5 Continue
!
! Decay differential equations with early branching terms set to zero
!  because we know we never skip more than 4 isotopes in a branch.
! In short, (blam i,j)=0 if i-j>5, so leave out those terms
!
       Do 20 i=1,n
         Do 10 j=1,i
           first(i)=first(i)+(blam(i,j)*yg(j))
   10    Continue
        ydotg(i)=first(i)-(lame(i)*yg(i))+deptot(i)
   20  Continue
! print*,"In f_gc, t is: ",t, "y1= ",y(1)


      RETURN
      END
```

Max of 30 members in chain

Sum of chain ingrowth terms

(Chain ingrowth) – removal + deposition

Numerical Methods Testing Results

Part of Alpha Phase testing:

Ground Concentration
- Solved the equations analytically for up to 6 members
- Programmed solution into Excel
- Tested against 5 member Sr-81 chain analytical with good agreement

Air Concentration
- Bateman equations with branching (no deposition or leaching)
- Tested against web solvers and Excel versions of analytical solution
- All tests showed good agreement

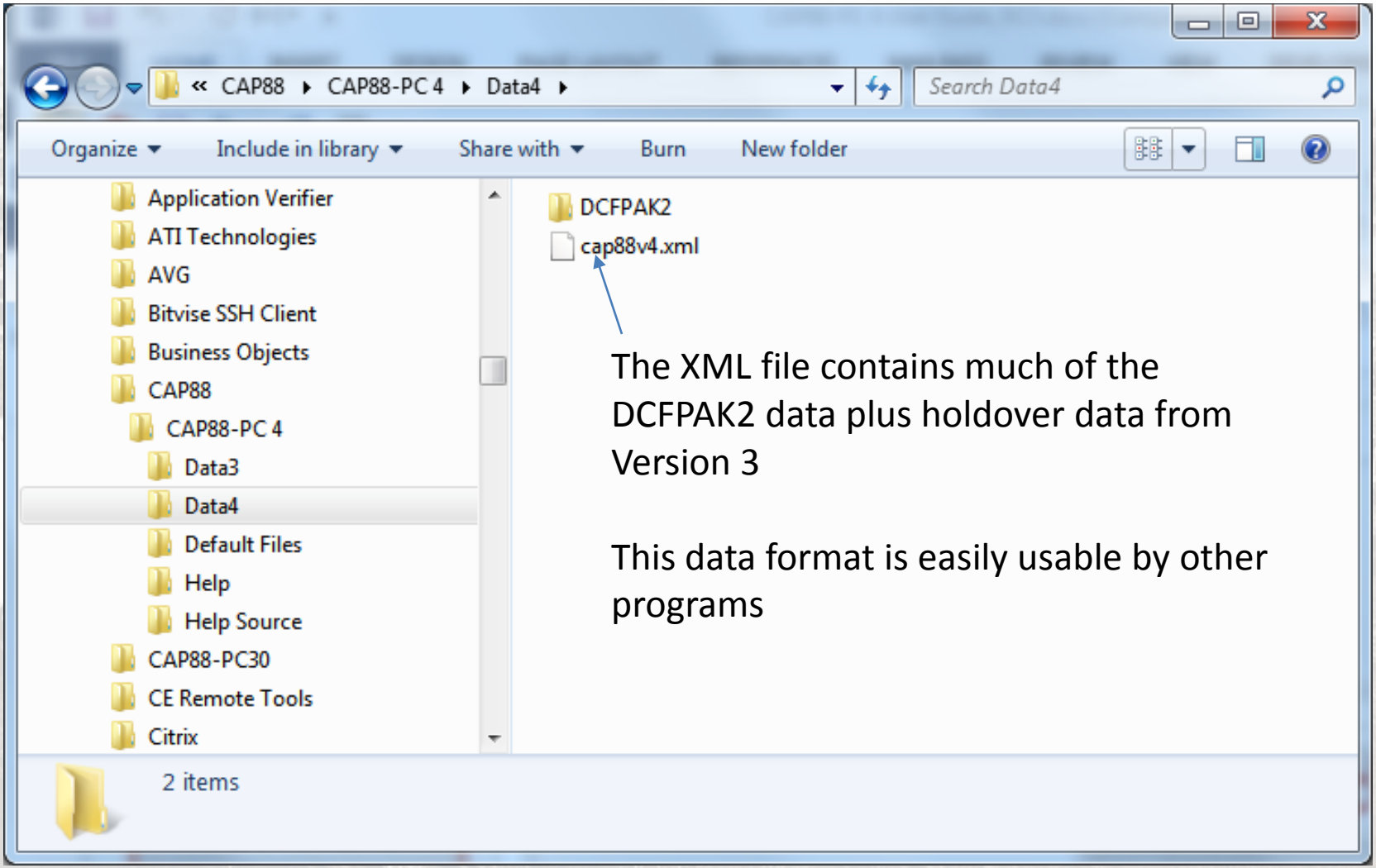
Tested solver for resiliency against stiff problems with good results

Example Alpha Phase Test Results

U-235 Chain, CAP88 Solver vs. On-line Decay Solver at WISE Uranium Project

	Cap88	WISE
Case4: 10,000 units U235, no daughters at t=0, 1000 y		
U-235	1.00E+04	1.00E+04
Th-231	1.00E+04	1.00E+04
Pa-231	2.09E+02	2.09E+02
Ac-227	2.03E+02	2.03E+02
Th-227	2.00E+02	2.00E+02
Fr-223	2.80E+00	2.80E+00
Ra-223	2.03E+02	2.03E+02
Rn-219	2.03E+02	2.03E+02
At-219	1.68E-04	
Bi-215	1.63E-04	
Po-215	2.03E+02	2.03E+02
Pb-211	2.03E+02	2.03E+02
Bi-211	2.03E+02	2.03E+02
Tl-207	2.02E+02	2.02E+02
Po-211	5.60E-01	5.68E-01

New Data Locations



The XML file contains much of the DCFPAK2 data plus holdover data from Version 3

This data format is easily usable by other programs

XML Data File State Ag Data

```
<?xml version="1.0" encoding="utf-8" standalone="yes"?>
<Data>
  <AgriData Type="System.Collections.Generic.List`1[[Cap88Pc.Data3.AgriData,
Cap88Pc, Version=4.0.0.0, Culture=neutral, PublicKeyToken=null]]">
    <Record>
      <StateName Type="System.String">Alabama</StateName>
      <StateAbbr Type="System.String">AL</StateAbbr>
      <BeefDensity Type="System.Decimal">0.1520</BeefDensity>
      <MilkDensity Type="System.Decimal">0.007020</MilkDensity>
      <VegetationDensity Type="System.Decimal">0.004160</VegetationDensity>
    </Record>
```

XML Data File Isotope data

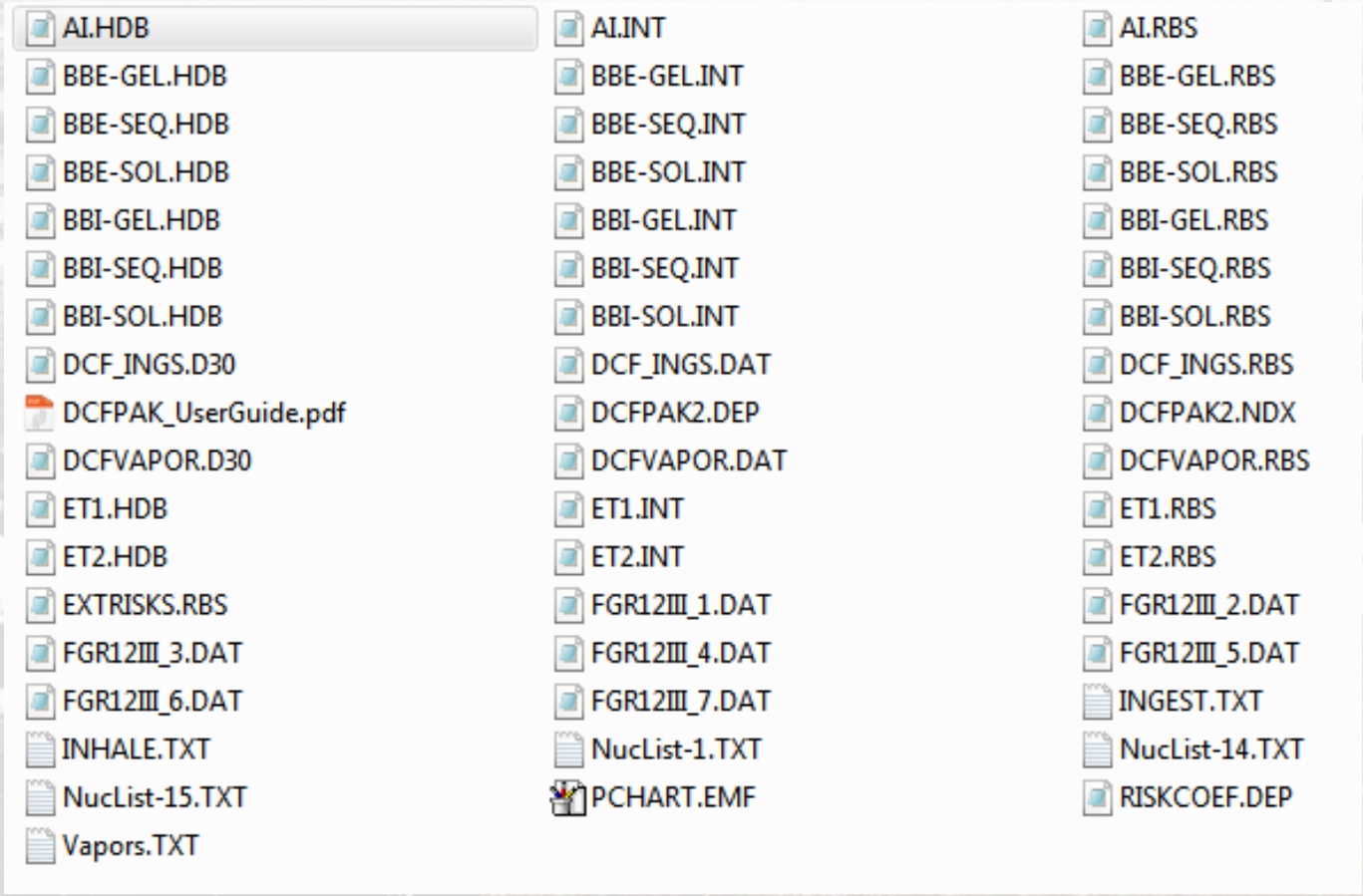

```
<NuclideIndex Type="System.Collections.Generic.List`1[[Cap88Pc.Data4.NuclideIndex, Cap88Pc,
Version=4.0.0.0, Culture=neutral, PublicKeyToken=null]]">
  <Record>
    <NuclideName Type="System.String">Ac-223</NuclideName>
    <HalfLife Type="System.Decimal">2.10</HalfLife>
    <HalfLifeUnit Type="System.String">m</HalfLifeUnit>
    <Fgr12iiiDat Type="System.Int32">1116</Fgr12iiiDat>
    <ExtRisksRbs Type="System.Int32">16684</ExtRisksRbs>
    <DcfIngsDat Type="System.Int32">0</DcfIngsDat>
    <DcfIngsRbs Type="System.Int32">0</DcfIngsRbs>
    <DcfIngsD30 Type="System.Int32">0</DcfIngsD30>
    <IngestionChemicalForms Type="System.Int32">0</IngestionChemicalForms>
    <Hdb Type="System.Int32">0</Hdb>
    <Rbs Type="System.Int32">0</Rbs>
    <D30 Type="System.Int32">0</D30>
    <InhalationChemicalForms Type="System.Int32">0</InhalationChemicalForms>
    <DcfVaporDat Type="System.Int32">0</DcfVaporDat>
    <DcfVaporRbs Type="System.Int32">0</DcfVaporRbs>
    <DcfVaporD30 Type="System.Int32">0</DcfVaporD30>
    <VaporGasChemicalForms Type="System.Int32">0</VaporGasChemicalForms>
  </Record>
```

XML Data File Chain Data

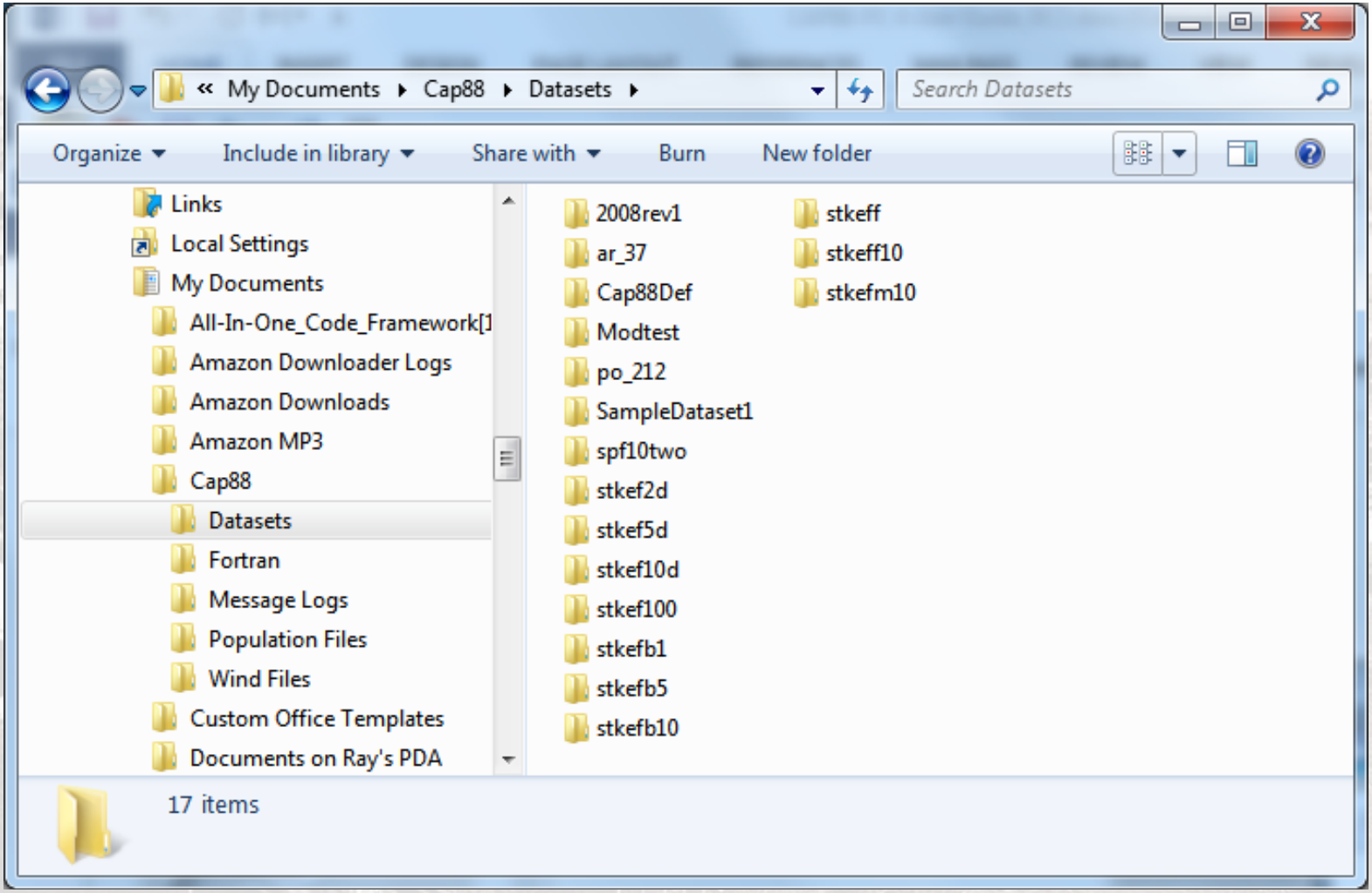

```
<DcfDecayParent Type="System.Collections.Generic.List`1[[Cap88Pc.Data4.DcfDecayParent, Cap88Pc, Version=4.0.0.0,
Culture=neutral, PublicKeyToken=null]]">
  <Record>
   <NuclideName Type="System.String">Ne-24</NuclideName>
   <DecayItems Type="System.Collections.Generic.List`1[[Cap88Pc.Data4.DcfDecayItem, Cap88Pc, Version=4.0.0.0, Culture=neutral,
PublicKeyToken=null]]">
    <Record>
     <NuclideName Type="System.String">Ne-24</NuclideName>
     <Daughters Type="System.Collections.Generic.List`1[[Cap88Pc.Data4.DcfDecayItemDaughter, Cap88Pc, Version=4.0.0.0,
Culture=neutral, PublicKeyToken=null]]">
      <Record>
       <NuclideName Type="System.String">Na-24</NuclideName>
       <DecayPercent Type="System.Decimal">1.000</DecayPercent>
       <IsFinalItem Type="System.Boolean">false</IsFinalItem>
      </Record>
     </Daughters>
    </Record>
    <Record>
     <NuclideName Type="System.String">Na-24</NuclideName>
     <Daughters Type="System.Collections.Generic.List`1[[Cap88Pc.Data4.DcfDecayItemDaughter, Cap88Pc, Version=4.0.0.0,
Culture=neutral, PublicKeyToken=null]]">
      <Record>
       <NuclideName Type="System.String">Mg-24</NuclideName>
       <DecayPercent Type="System.Decimal">1.000</DecayPercent>
       <IsFinalItem Type="System.Boolean">true</IsFinalItem>
      </Record>
     </Daughters>
    </Record>
   </DecayItems>
  </Record>
```

DCFPAK V2.2 Data Source

Included with installation package under installed program folder



New Dataset Location



V4 Dataset File Structure

Editable Text Format, but Direct Editing NOT Advised

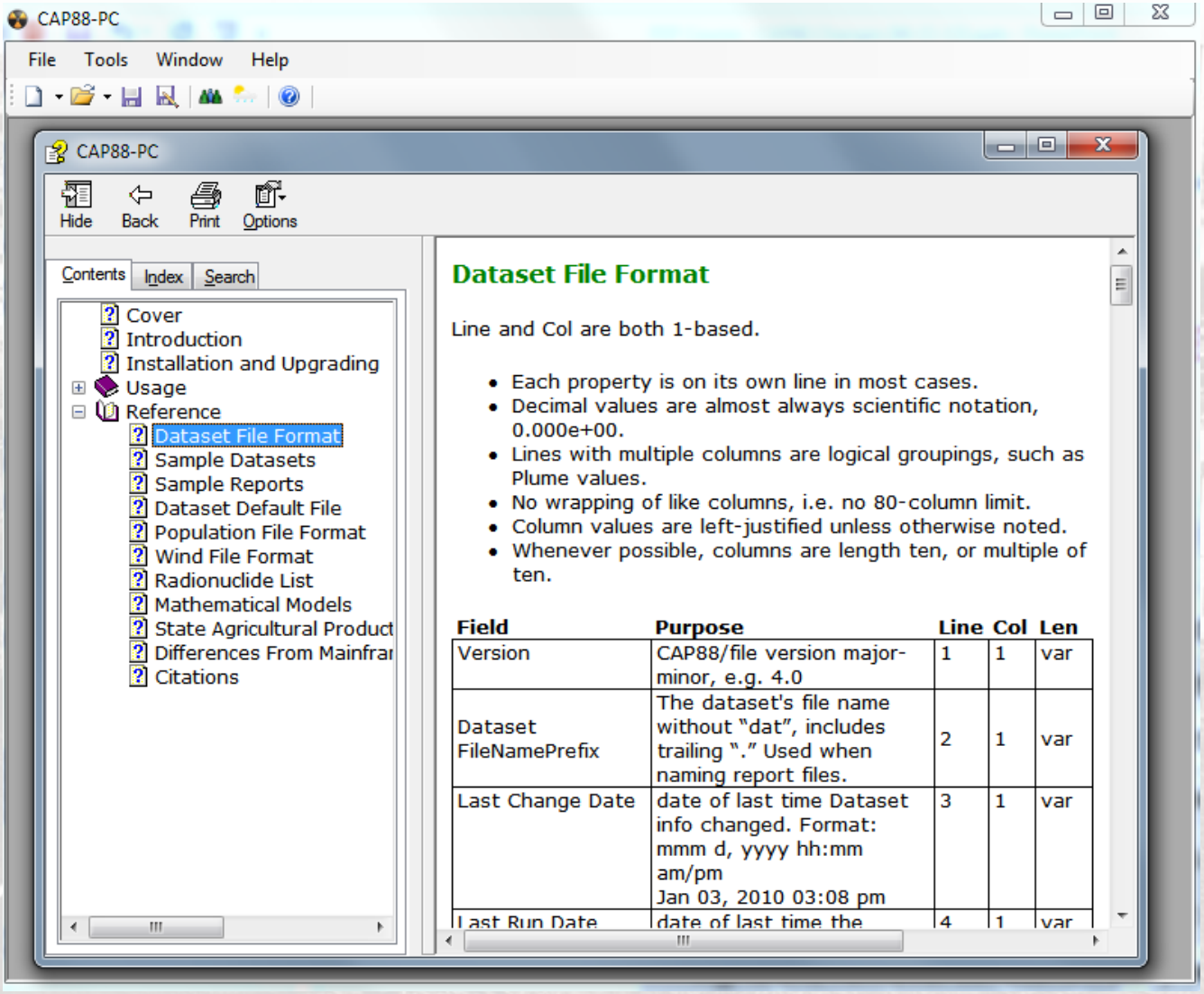
po_212.dat - Notepad

File Edit Format View Help

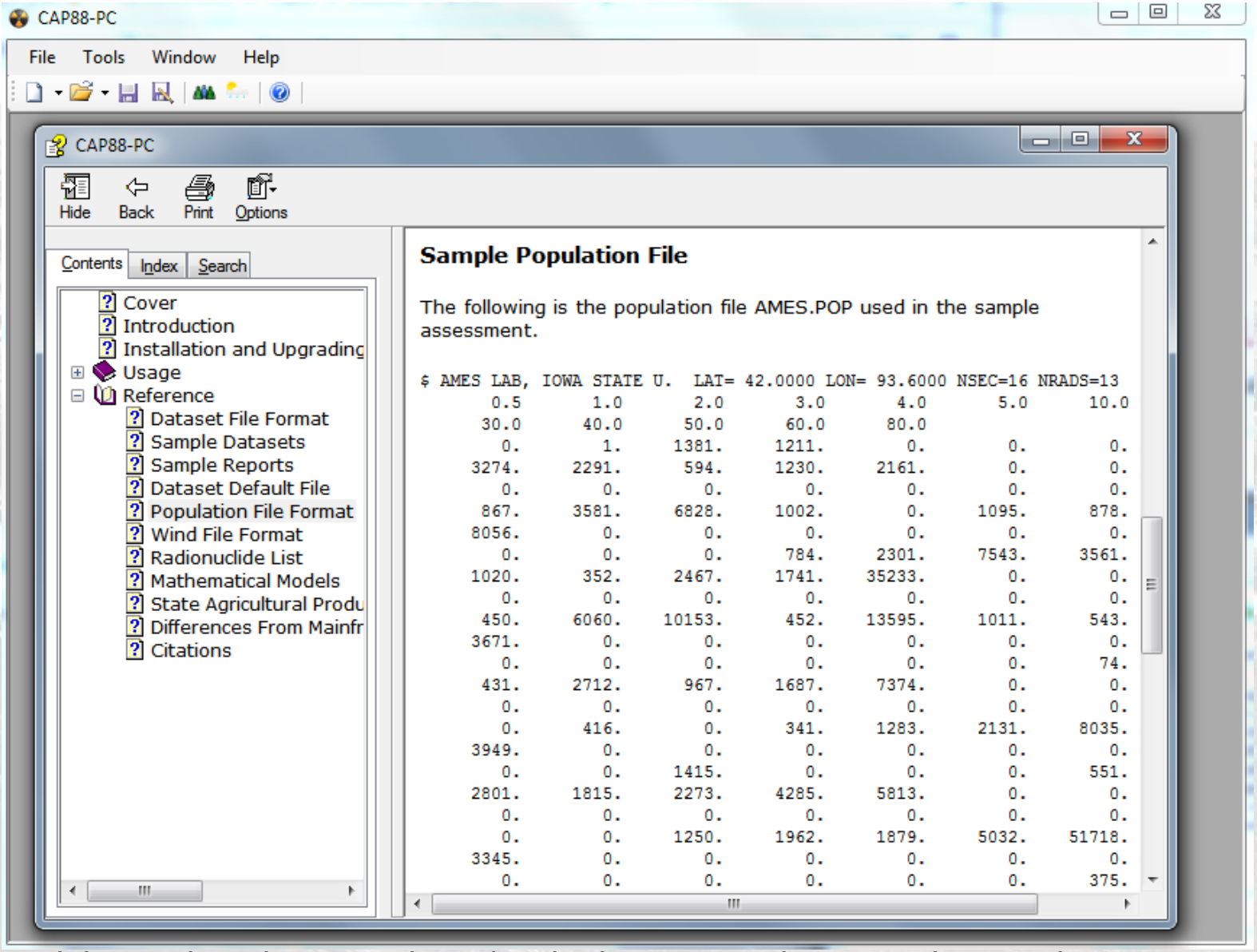
```
4.0
Po_212.
Jan 25, 2013 08:36 PM
Jan 25, 2013 08:36 PM
Der Test Haus
8832 Falmouth Dr

Cincinnati
45231
old 3 stack
2010
1, 2, 3, Ci K-40
Avg Met
1
C:\Program Files (x86)\CAP88-PC30\PopFiles\FERMILAB.POP
Adult
100
13
0
0
250       750       1500      2500      3500      4500      7500      15000     25000     35000     45000     55000     70000     0         0         0         0         0
T         T         T         T
C:\Program Files (x86)\CAP88-PC30\WndFiles\03816.WND
40.00
6.01
800.00
8.00
0
3
1.000e+00 1.000e+00 1.000e+00
1.000e+00 1.000e+00 1.000e+00
0
1.500e+00 1.500e+00 1.500e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00
1
0.70      0.30      0.00
0.40      0.60      0.00
0.44      0.56      0.00
OH
2.030e-01
4.560e-02
1.700e-02
86400
5
F
1
0         K-40      Particulate                         M         1.0000    1.000e+00 2.000e+00 3.000e+00
84        93        53        84        493       5263
Adrenal   UB_Wall   Bone_Sur  Brain     Breasts   St_Wall   SI_Wall   ULI_Wall  LLI_Wall  Kidneys   Liver     Muscle    Ovaries   Pancreas  R_Marrow  Skin      Spleen    Testes
esophagus stomach   colon     liver     lung      bone      skin      breast    ovary     bladder   kidney    thyroid   leukemia  residual  Total
1
K-40      Particulate                         M         1.0000    3.948e+16 1.800e-03 1.000e-07 5.480e-05 1.000e+00 1.000e+00 2.000e-02 7.000e-03 3.000e-01 3.000e+00
0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e+00 0.000e
5.040e-09 6.270e-09 5.000e-09 4.860e-09 4.830e-09 5.590e-09 5.100e-09 9.700e-09 1.880e-08 5.000e-09 5.000e-09 4.940e-09 5.110e-09 5.060e-09 4.960e-09 4.800e-09 5.000e-09 4.940e
1.731e-09 1.829e-09 1.565e-09 1.438e-09 1.706e-09 1.715e-09 1.511e-09 2.845e-09 5.434e-09 1.555e-09 1.690e-09 1.553e-09 1.501e-09 1.664e-09 1.588e-09 1.461e-09 1.655e-09 1.437e
6.650e-15 6.760e-15 1.120e-14 8.520e-15 8.860e-15 7.160e-15 6.620e-15 6.780e-15 6.700e-15 7.180e-15 7.260e-15 7.730e-15 6.810e-15 6.550e-15 7.870e-15 4.190e-14 7.270e-15 7.830e
1.260e-16 1.420e-16 1.940e-16 1.340e-16 1.450e-16 1.360e-16 1.360e-16 1.360e-16 1.400e-16 1.380e-16 1.370e-16 1.520e-16 1.280e-16 1.290e-16 1.460e-16 6.230e-15 1.360e-16 1.520e
2.480e-13 3.480e-12 5.430e-12 3.700e-13 2.370e-12 2.270e-14 1.940e-14 9.660e-13 3.350e-13 6.350e-13 1.280e-13 8.290e-14 1.300e-12 4.190e-12 1.960e-11
1.474e-12 2.534e-12 8.805e-12 1.906e-12 4.184e-10 1.063e-13 7.601e-14 2.783e-12 1.458e-12 3.422e-12 5.988e-13 1.851e-13 6.839e-12 8.935e-12 4.575e-10
7.900e-18 2.890e-17 6.960e-17 1.100e-17 7.750e-17 1.060e-18 4.180e-18 4.280e-17 9.690e-18 1.630e-17 3.740e-18 2.570e-18 4.420e-17 1.040e-16 4.230e-16
1.420e-19 5.490e-19 1.420e-18 2.080e-19 1.390e-18 1.840e-20 6.220e-19 7.010e-19 1.820e-19 3.430e-19 7.180e-20 4.360e-20 8.200e-19 2.020e-18 8.530e-18
```

Dataset File Description

Contained in User Manual Accessible Via Help Button



Population File Structure



WIND FILE STRUCTURE

03160_WND_Documented.txt - Notepad

File Edit Format View Help

```
 ┐└ [Magic Value]
   4.27363 [Average Wind Speed]
0.05900.01810.03940.07870.08100.06820.12380.09540.06090.02820.02530.02410.03750.06360.10320.0936 [Wind Direction Frequency;| Sum to 1]
 1.33 1.11 1.27 1.15 1.08 1.35 1.36 1.50 1.13 1.25 1.47 1.10 1.25 1.36 1.41 1.45 [Pasquill A Reciprocal Average Wind Speed Toward Direction N-NNE]
 1.47 1.33 1.25 1.38 1.25 1.39 1.33 1.50 1.45 1.24 1.34 1.23 1.51 1.71 1.85 1.62
 3.12 2.18 2.68 2.64 2.24 2.51 3.28 3.07 2.65 1.92 1.91 2.00 2.68 3.66 4.09 4.17
 6.07 3.43 4.29 4.77 4.19 4.69 6.02 5.91 4.68 3.68 3.25 3.42 3.87 5.17 6.15 6.89
 3.61 3.13 3.22 3.49 3.34 3.52 3.82 3.78 3.34 3.28 3.10 3.18 3.39 3.70 3.89 3.81
 1.26 1.24 1.26 1.39 1.38 1.38 1.40 1.43 1.34 1.35 1.14 1.17 1.28 1.36 1.37 1.20
 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 [Pasquill G Reciprocal Average Wind Speed Toward Direction N-NNE]
 1.85 1.56 1.78 1.62 1.50 1.87 1.88 2.02 1.59 1.76 1.99 1.53 1.75 1.89 1.94 1.97 [Pasquill A True Average Wind Speed Toward Direction N-NNE]
 2.32 2.16 2.04 2.30 2.00 2.22 2.05 2.47 2.27 1.97 2.08 1.91 2.33 2.67 2.80 2.59
 4.92 3.23 3.66 3.84 3.39 3.44 4.17 4.12 3.67 2.88 2.78 2.84 3.58 4.66 5.45 5.69
 7.10 4.59 5.22 5.56 5.30 5.76 6.61 6.68 6.01 5.20 4.81 4.64 5.00 5.99 6.97 7.68
 3.83 3.35 3.45 3.72 3.57 3.75 4.00 3.97 3.58 3.52 3.32 3.41 3.63 3.91 4.05 4.00
 1.77 1.74 1.76 1.91 1.90 1.90 1.93 1.96 1.87 1.87 1.60 1.65 1.79 1.88 1.89 1.68
 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 [Pasquill G True Average Wind Speed Toward Direction N-NNE]
    0.0147    0.0903    0.1610    0.4659    0.1289    0.1392    0.0000 [Fraction of Time in Pasquill Category A-G Direction N]
    0.0177    0.1546    0.1866    0.2087    0.1160    0.3164    0.0000 [Fraction of Time in Pasquill Category A-G Direction NNW]
    0.0041    0.0921    0.1707    0.3293    0.1347    0.2692    0.0000
    0.0048    0.0441    0.0980    0.3522    0.1750    0.3258    0.0000
    0.0064    0.0468    0.0757    0.2085    0.1890    0.4736    0.0000
    0.0072    0.0419    0.0629    0.2029    0.2365    0.4486    0.0000
    0.0021    0.0247    0.0604    0.4410    0.2253    0.2465    0.0000
    0.0024    0.0343    0.0926    0.4362    0.1943    0.2402    0.0000
    0.0076    0.0765    0.1248    0.2351    0.1912    0.3649    0.0000
    0.0149    0.1377    0.1360    0.2001    0.1512    0.3601    0.0000
    0.0269    0.1766    0.1797    0.1971    0.1342    0.2854    0.0000
    0.0295    0.2431    0.2003    0.1816    0.1222    0.2232    0.0000
    0.0181    0.2258    0.2490    0.2474    0.1017    0.1580    0.0000
    0.0157    0.1323    0.2612    0.3845    0.1053    0.1009    0.0000
    0.0069    0.0772    0.2351    0.5318    0.0916    0.0574    0.0000
    0.0051    0.0742    0.1790    0.6065    0.0828    0.0525    0.0000 [Fraction of Time in Pasquill Category A-G Direction NNE]
extended data
StationName=DESERT ROCK
State=NV
Latitude=36.617
Longitude=116.017
TimeZone=8
RecordPeriod=1988,1989,1990,1991,1992
AveragePeriodTemperature=17.64
Comments=
```

Wind file editor is still being developed