Annex IV

A Description of the Model Equations

B Distributions Intomart Database

C Simulation of the Time Fractions in the *EXPOLIS* model

A Description of model equations

input - *Input (sub)population sheet*

Cells C8-C19	Names of microenvironments (μE) with known concentration distribution that will be used in the model; the user is free to select his own μEs with a maximum of 12. Required, text.
Cells D8-D19	Mean of the concentration distribution in each μE (C_i) with known concentration distribution. A lognormal distribution is assumed. Required if μE defined, number (>0), μg/m^3.
Cells E8-E19	Standard deviation of the concentration distribution in each μE. A lognormal distribution is assumed. Required if μE defined, number (>0), μg/m^3.
Cells F8-F19	Mean of fractional time in each μE (f_i). A beta distribution is assumed. Should be entered as a fraction of 1. Required if μE defined, number (Between 0 and 1).
Cells G8-G19	Standard deviation of fractional time in each μE. A beta distribution is assumed. Required if μE defined, number (>0).
Cells C26-C33	Names of microenvironments (μE) with unknown concentration distribution that will be used in the model; the user is free to select his own μEs with a maximum of 8. Not required, text.
Cells D26-D33	Mean of fractional time in each μE (f_i). A beta distribution is assumed. Should be entered as a fraction of 1. Required if μE defined, number (Between 0 and 1), percentage
Cells E26-E33	Standard deviation of fractional time in each μE. A beta distribution is assumed. Required if μE is defined, number (>0).
Cells F26-F33	Mean of penetration factor or Input/Output value (p_i). A beta distribution is assumed. Required if μE is defined, percentage of outdoor conc. (between 0 and 1)
Cells G26-G33	Standard deviation of penetration factor. A beta distribution is assumed. Required if μE is defined, number
Cells H26-H33	Indicate the outdoor μE that should be used for estimation of the concentration distribution. Should be selected from list in cells C8-C19. Required if μE is defined, integer (1-12).
Cells I26-M33	Possibility to add indoor sources to estimation of concentration distribution. Possible to add a maximum of 5 indoor sources. These columns also say something about the occurrence of the indoor sources in the population (for example, 40% of the population is smoking when the value 0.4 is entered) Not required, number between 0 and 1.

Cell D34	Sum of fractional times in cells F8-F19 and D26-D33. Should add up to 1.
Cells C40-C44	Names of indoor sources (S_n) that will be entered into the model. A maximum of 5 indoor sources is possible. Not required, text.
Cells D40-D44	Mean of the concentration distribution of an indoor source. A lognormal distribution is assumed. Required if indoor source is defined, number (>0), μg/m^3.
Cells E40-E44	Standard deviation of the concentration distribution of an indoor source. A lognormal distribution is assumed. Required if indoor source is defined, number, μg/m^3.

Correction - *Correlation matrix*

Cells D4-AV4 and C5-C49

Names of μE's, repeated from input sheet.

Cells D5-AV49	Correlation matrix. Not required, values between -1 and 1.

Calculation - *Calculation sheet 1*

Cells C8-C19	='input'!C8 Repeat names of μEs on calculation sheet
Cells D8-D19	=IF('input'!F8>0,((('input'!F8^2)/('input'!G8^2))*((1-'input'!F8)/'input'!F8)-1)/(1+((1-'input'!F8)/'input'!F8)),0) Calculation of 'α1' for beta distribution fractional time for known concentration distributions.
Cells E8-E19	=IF('input'!F8>0,D8*((1-'input'!F8)/'input'!F8),0) Calculation of 'α2' for beta distribution fractional time.
Cells F8-F19	=IF('input'!F8>0,RiskCorrmat('correlation'!$D$5: 'correlation'!$AV$49,21)+RiskBeta(D8,E8),0) Calculation of beta distribution fractional time based on column D and E (for known concentration distributions).
Cells G8-G19	=F8/$F$35 Divide sampled time fraction by total sampled time fraction
Cells H8-H19	=IF('input'!D8>0,RiskCorrmat('correlation'!d5: 'correlation'!$AV$49,1)+RiskLognorm('input'!D8,'input'!E8),0) Calculation of the concentration distribution for each μE based on a lognormal distribution, including possible correlations.
Cells P8-P19	=IF(ISERROR(H8)=FALSE,(G8*H8),0)

Calculation of the fractional concentration in the μEs with known concentration distribution

Cells C26-C33	='input'!C26 Repeat names of μEs on calculation sheet
Cells D26-D33	=IF('input'!D26>0,((('input'!D26^2)/('input'!E26^2))*((1-'input'!D26)/'input'!D26)-1)/(1+((1-'input'!D26)/'input'!D26)),0) Calculation of 'α1' for beta distribution fractional time for unknown concentration distributions
Cells E26-E33	=IF('input'!D26>0,D26*((1-'input'!D26)/'input'!D26),0) Calculation of 'α2' for beta distribution fractional time.
Cells F26-F33	=IF('input'!D26>0, RiskCorrmat('correlation'!$D$5:'correlation'!$AV$49,33)+RiskBeta(D26,E26),0) Calculation of beta distribution fractional time based on column D and E (for unknown concentration distributions).
Cells G26-G33	=F26/$F$35 Divide sampled time fraction by total sampled time fraction
Cells H26-H33	=IF('input'!F26>0,((('input'!F26^2)/('input'!G26^2))*((1-'input'!F26)/'input'!F26)-1)/(1+((1-'input'!F26)/'input'!F26)),0) Calculation of 'α1' for beta distribution penetration factor for unknown concentration distributions
Cells I26-I33	=IF('input'!F26>0,H26*((1-'input'!F26)/'input'!F26),0) Calculation of 'α2' for beta distribution penetration factor
Cells J26-J33	=IF('input'!F26>0, RiskCorrmat('correlation'!$D$5:'correlation'!$AV$49,13)+RiskBeta(H26,I26),0) Calculation of beta distribution penetration factor based on column D and E.
Cells K26-K33	=SUM((ROUNDUP(D42,0)*F$40*F42),(ROUNDUP(H42,0)*J$40*J42),(ROUNDUP(K42,0)*M$40*M42),(ROUNDUP(N42,0)*P$40*P42),(ROUNDUP(Q42,0)*S$40*S42)) Summing the contribution of indoor sources. The formula for each indoor source is: indoor source present (yes/no using the function roundup) times concentration distribution of source times percentage of population exposed to the source (using a discrete distribution).
Cells L26-L33	='input'!H26 Repeat indicator for outdoor μE that should be used for estimation.
Cells M26-M33	=H8 Concentration distribution of C_{out}, implemented using the macro ***dcout*** that is run before the model simulation starts running.
Cells N26-N33	=M26*J26+K26 Calculation of estimation of concentration distribution C_i.

Cells P26-P33 =IF(ISERROR(N26)=FALSE,(G26*N26),0)
Calculation of the fractional concentration in the μEs with unknown concentration distribution

Cell D35 =sum(F8:F19,F26:F33)
Total sum of sampled time fractions

Cells D42-D49, cells H42-H49, cells K42-K49, N42-N49, Q42-Q49
='input'!I26
Percentage of the population exposed to a certain indoor source, for each indoor source coupled to each μE.

Cells E42-E49, cells I42-I49, cells L42-L49, O42-O49, R42-R49
=1-D42
Percentage of the population that is <u>not</u> exposed to a certain indoor source, for each indoor source coupled to each μE.

Cells F42-F49, cells J42-J49, cells M42-M49, P42-P49, S42-S49
=IF(D42>0,RiskDiscrete({1,0},D42:E42),0)
Calculate percentage of population that is exposed to a certain indoor source using the discrete distribution

Cells F40, J40, M40, P40, S40
=IF('input'!D40>0, RiskCorrmat('correlation'!$D$5:'correlation'!$AV$49,41)+RiskLognorm('input'!D40,'input'!E40),0)
Calculate the lognormal distribution of the indoor sources.

Cell S33 =SUM(P8:P19,P26:P33)
The contribution of each μE is added up in cell S33. This cell is the output cell during the @Risk simulation of the model.

Macro dcout

```
'
' macro dcout
' determines which outdoor source contributes to indoor conc.
' macro recorded 13-1-98 by OBr
'

Sub dcout()
  For i = 26 To 33
    Worksheets("calculation").Activate
    Select Case Cells(i, 11).Value
      Case 1
        Cells(i, 12).Formula = "=G8"
      Case 2
        Cells(i, 12).Formula = "=g9"
      Case 3
        Cells(i, 12).Formula = "=g10"
      Case 4
        Cells(i, 12).Formula = "=g11"
      Case 5
        Cells(i, 12).Formula = "=g12"
      Case 6
        Cells(i, 12).Formula = "=g13"
      Case 7
        Cells(i, 12).Formula = "=g14"
      Case 8
        Cells(i, 12).Formula = "=g15"
      Case 9
        Cells(i, 12).Formula = "=g16"
      Case 10
        Cells(i, 12).Formula = "=g17"
      Case 11
        Cells(i, 12).Formula = "=g18"
      Case 12
        Cells(i, 12).Formula = "=g19"
      Case Else
        Cells(i, 12) = ""
      End Select
    Next i
End Sub
```

B Distributions Intomart database

Microenvironments in the Intomart database

1 At home, kitchen
2 At home, not in the kitchen
3 At home, outdoors
4 Indoors, not at home
5 Outdoors, not at home, in city, in center
6 Outdoors, not at home, in city, not in center
7 Outdoors, not at home, not in city
8 Questionnaire not filled in

For each microenvironment the mean and standard deviation were calculated, as well as the kurtosis and skewness of the distribution. Please note that all calculations were only performed on the respondents that actually visited a microenvironment during the period of 24 hours. If a respondent did not visit a microenvironment, a missing was recorded instead of a zero value.
Then, Bestfit fitted all possible distribution types that were available in the software and ranked the resulting distributions according to goodness-of-fit (using the chi-square, kolmogorov-Smirnov and Anderson-Darling statistics). The results can be found in the following table.

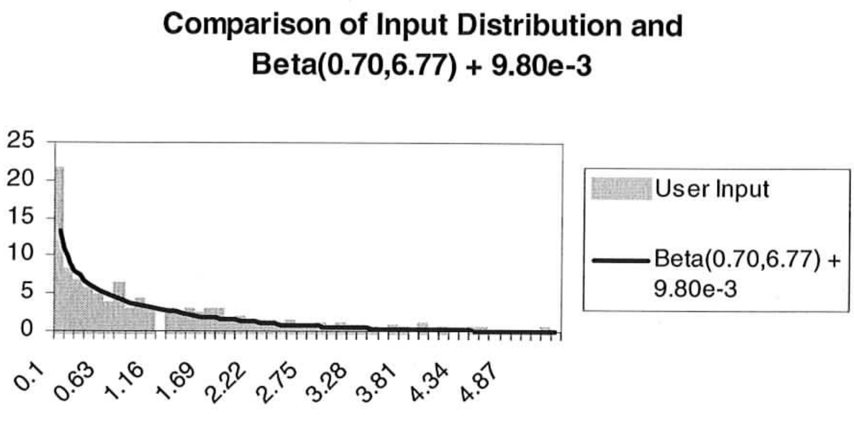
Selected type of distribution based on Bestfit results

Microenvironment	mean	std dev	Best distribution according to Bestfit	rank of beta distribution according to Bestfit
Home, kitchen	0.08	0.08	Pearson IV	17
Home, not kitchen	0.62	0.17	Logistic	10
Home, outside	0.11	0.10	Beta	1
Inside, not home	0.22	0.15	Weibull	16
Outside, city center	0.08	0.08	Beta	1
Outside, city, not center	0.09	0.09	InverseGaussian	5
Outside, not city	0.13	0.11	Lognorm	6

Examples of Bestfit output

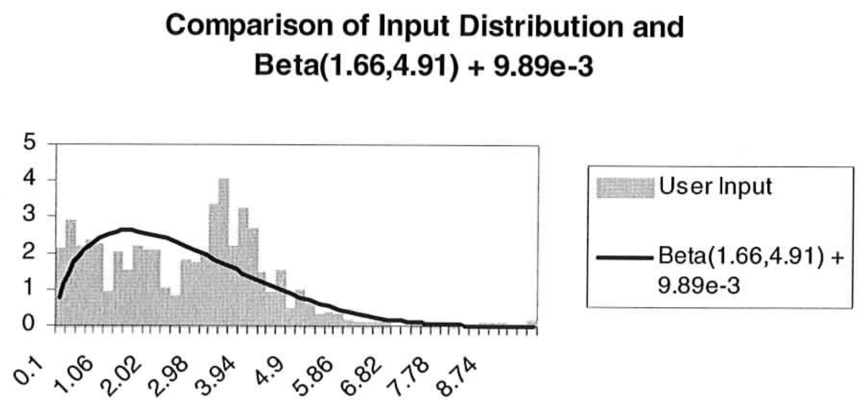
The following graph shows the results for microenvironment 3 (at home, outdoors). The columns show the input data from the intomart database and the line represent the beta distribution that Bestfit has fitted. The graph shows that the beta distribution seems to be a good choice for use in exposure modeling for the description of this particular microenvironment. However, it should be noted that Bestfit calculates a small shift to the right of the beta distribution. It is not possible to implement this shift in the current model.

Microenvironment 3: At home, outdoors



T not at home). Here it can be seen
t es any other type of distribution.
T ok at the microenvironment this
c :roenvironment can differ widely.
T ll in the same microenvironment.
T n under study and the
r der study.

M



C Simulation of time fractions in the *EXPOLIS* model

The sampling of the time fractions (f_i) deserves special attention because of a problem with the sum of the fractional times that is sampled during each iteration. This is best explained by a simple example.

Imagine a model with 2 µE's: outdoors and indoors, with the following parameters for the time fractions:

µE	time fraction (f_i)	first iteration	second iteration
Outdoors	0.2 (0.1)	0.35	0.15
Indoors	0.8 (0.2)	0.85	0.75
Total time	1.0	1.4	0.9

The table shows that the mean sum of the partial time fractions is 1. The problem arises when the simulation is run. In the table the sampling of the first and second iteration is shown. Because @Risk samples the partial time fractions from both µEs independently, the total sampled time can be larger or smaller than 1. For the total population this is no problem because the mean total time after a large number of iterations is approximately 1, but for each individual in the population (each iteration=1 individual) this gives a distortion. The resulting output distribution will change shape because of this problem.

We could find 3 possible solutions to solve the problem:

1. Sample partial time fractions from all but one µE during each iteration. The µE with the largest mean time fraction is not sampled and used to fill the gap between sum of the other time fractions and 1, according to the following formula:

   $f_x = 1 - \Sigma f_i$ where: f_i = time fraction spend in *i*-th microenvironment
   f_x = time fraction spent in microenvironment with largest mean time fraction

2. Divide each sampled time fraction by the total sum of the time fractions. In formula:

   Partial time fraction = f_i/f_i

3. Divide the resulting partial concentration by the total sum of the time fractions. In formula:

4. Partial concentration = $(C_i * f_i)/f_i$

Each solution has his own advantages and disadvantages. We checked the modeling results of all options. The first solution did not prove to be a useful option because it gave negative values for the time fraction in f_x in some iterations. The difference in the final results of solution 2 and 3 is small. We finally opted for solution 2 because it still offers the possibility to analyze the partial concentrations in your model.