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A Web Application to Investigate the Effects of Pollutants on Cetacean Populations (SPOC - Pollution 2020)

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INTERNATIONAL
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ABSTRACT

The risk assessment framework for evaluating the population consequences of pollutant exposure in cetaceans that has been developed as part of the IWC Pollution 2000+ and 2020 initiatives (Hall et al, (2011) SC/63/E5; Hall et al, (2014) SC64/E5; Hall et al, (2013) SC/E65A/E4) has been refined and made available as an on-line web application. Before general release, the model will be finally 'tested' by a number of researchers at the IWC Scientific Committee Meeting in 2015 to ensure there are no additional errors that need to be rectified. The application is based on a framework that combines an individual-based model with concentration (dose)-response functions to estimate the effect of pollutants on a population's potential growth rate. The approach can then be applied to any cetacean population of interest, provided some basic information about the dynamics of that population is available. Its flexibility allows the user, through a user-input interface described in this paper, to (i) modify the starting population (using different vital rates relevant for the cetacean population of interest), (ii) choose which physiological effects of contaminant exposure they wish to focus on (currently parameterised with the effects of polychlorinated biphenyls (PCBs) on offspring survival probability or offspring survival probability and immunity) and (iii) examine the model outputs in the form of simulated potential population growth rates and final concentrations of PCBs in the adult females. Documentation on how to use the application is also downloadable from the interface to complement the shorter instructions given in the application itself.

Additional work, such as incorporating the effects of polycyclic aromatic hydrocarbons on cetacean health and survival, is currently underway. However, because these compounds are not accumulated and depurated in the same way as the persistent organic pollutants, a modification to the basic model framework is required.

Introduction

This web application is available from the link <http://www.smru.st-andrews.ac.uk/PCBdemo/> and the password will be made available in the first instance to researchers at the IWC Scientific Committee meeting. The researchers will be able to 'test' run the programme and any errors will be rectified before the application is made more generally available. Details of the background and development of the model framework are available in a number of publications (Hall et al. 2006, 2011, 2012, 2013) and these are downloadable through the application interface from the landing page, in addition to the more specific guidance documentation. Here we describe the user-interface for the application, with screen shots to illustrate the model process and various steps involved.

The application allows the user, through a set of input boxes or sliders, to:

1. Set up a baseline population for a cetacean species at risk, using a standard Leslie Matrix model. This generates a starting population for the application with a stable age structure. Users need to therefore decide on the vital rates that should be used to generate a population, preferably using data for the specific species and location of particular interest.

2. Generate concentration (dose) – response functions using data from cetaceans (where available) combined with data from laboratory animal models. The response functions currently embedded include
 - (a) investigating the effect of maternal polychlorinated biphenyls (PCBs) on calf survival and
 - (b) assessing the effect of PCBs on immunity and survival following exposure to a pathogen.
3. Run a set of simulated population trajectories, generated from an individual based model (with uncertainty), to estimate the effect of PCBs, through the dose-response relationships selected, on the potential population growth rates. The model runs for 100 years and the growth rates from years 60 to 95 are calculated. The user can simulate the effect of different levels of annual accumulation of PCBs (exposures) and can determine the effect of decreasing accumulation concentrations (the level of decrease is also chosen by the user) after year 50. If immune effects are also included in the model, the proportion of the population additionally exposed to a pathogen (either a low or higher virulence pathogen) can also be varied by the user. Of course, the baseline survival rates will already include any effects that infectious disease has on the population as part of the natural mortality drivers, but here we explore the effect of introducing a novel pathogen into the population. And by exposing a high proportion of the population, the impact of an epidemic can be investigated.
4. Plot the population growth rates and save these results for further analysis.
5. Plot the concentrations of PCBs in the adult females and save these concentrations for comparison with empirical data.

The program currently runs as a demonstration on a server at the Sea Mammal Research Unit. This will allow researchers to test the application and suggest additional changes that are required (either in the short term or in future). Once this final round of testing is complete, the application will be available for general use. The code itself will also be made available for researchers to make bespoke changes to the programme, for example additional dose-response functions could be added and the effects of different POP contaminants tested.

User Interface

The following set of screen shots shows the various tabs (listed above) and how the user can modify the various parameters.

The 'About' Tab

The landing page gives an introduction to the application (Fig. 1). It describes the various model sections and tabs and gives a link to where further documentation about SPOC can be found.

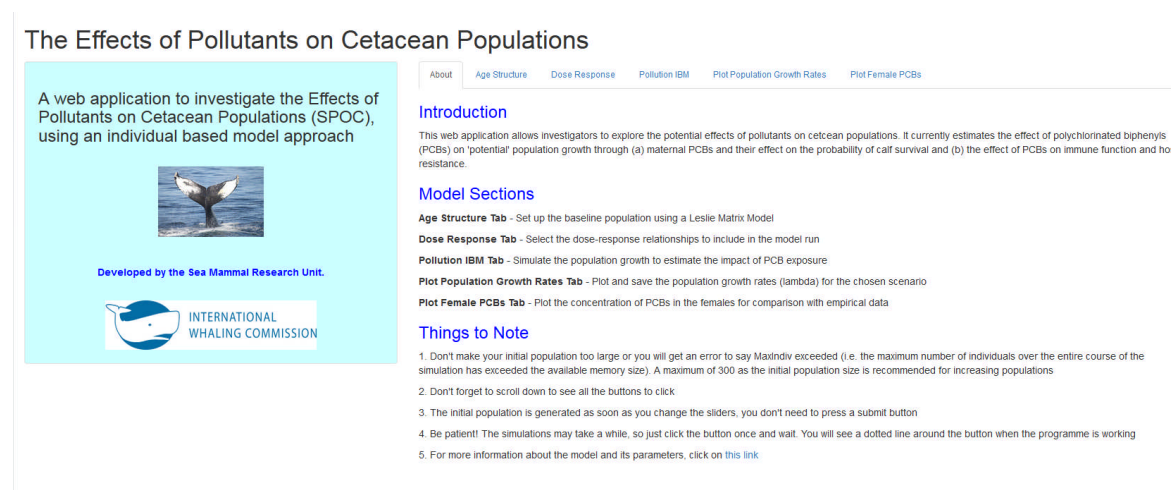


Figure 1. The 'About' tab and landing page.

The Age Structure Tab

The second tab allows the user to set up the starting population (Fig. 2). For this they need to provide information on

1. Calf survival (0 to 1 year old).

2. Juvenile survival (>1 year old to age at sexual maturity).
3. Reproductive female survival (from age at sexual maturity to reproductive senescence).
4. Post reproductive female survival (if unknown, this should be set at the same value as the reproductive female survival).
5. Female fecundity. This is modified in the programme to reflect the fact that this is a female only population. The sex ratio at birth is assumed to be 1:1 male to female.
6. Maximum age.
7. Female age at sexual maturity (i.e. age at first reproduction).
8. Female post reproductive age (this could be the same as maximum age if there is no reproductive senescence).
9. Initial population size. For a growing population this should not be too large (a maximum of 300 individuals but 100 would be recommended. But for declining populations this could be increased) otherwise the maximum number of individuals the application can model will be exceeded and will generate an error message.

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Figure 2. This age-structure interface sets up the starting population and allows the user to investigate the effect of PCBs on populations with different vital rates.

The Dose Response Tab

This interface generates the concentration (dose)-response relationships that are used to modify survival. In the current version this comprises two functions. Here the term dose is used as this is common terminology but in this context it refers to the level of contaminants in the blubber and the uptake of PCBs rather than an ingested concentration or 'dose' as commonly used in toxicology studies.

(i) Effects of maternal PCBs on offspring survival (Fig. 3). This function is generated from data gathered from a number of different studies on the effects of maternal PCBs on the survival of mink in a variety of laboratory studies. There is insufficient data available from cetaceans for this to be a species-specific relationship but mink

studies have been used in human risk assessments because they are sensitive to the effects of PCBs. Further details of the data used are given in Hall et al. (2011), being largely collated from Fuchsman et al (2008).

These data were used because the concentrations of PCBs in mink adipose were reported which is comparable to the empirical data available for cetaceans which are generally blubber levels rather than ingested dose. The best fitting model is shown with confidence intervals (in dark grey) but in the model 500 bootstrapped relationships are generated and the simulation then uses one of these relationships, chosen at random, to capture the uncertainty in this relationship.

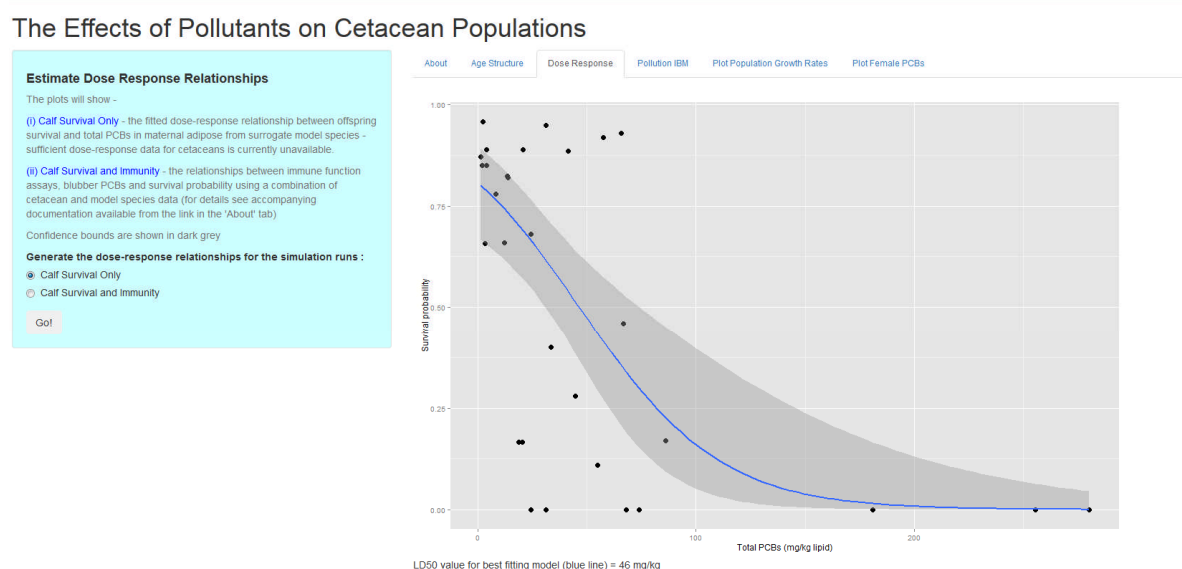


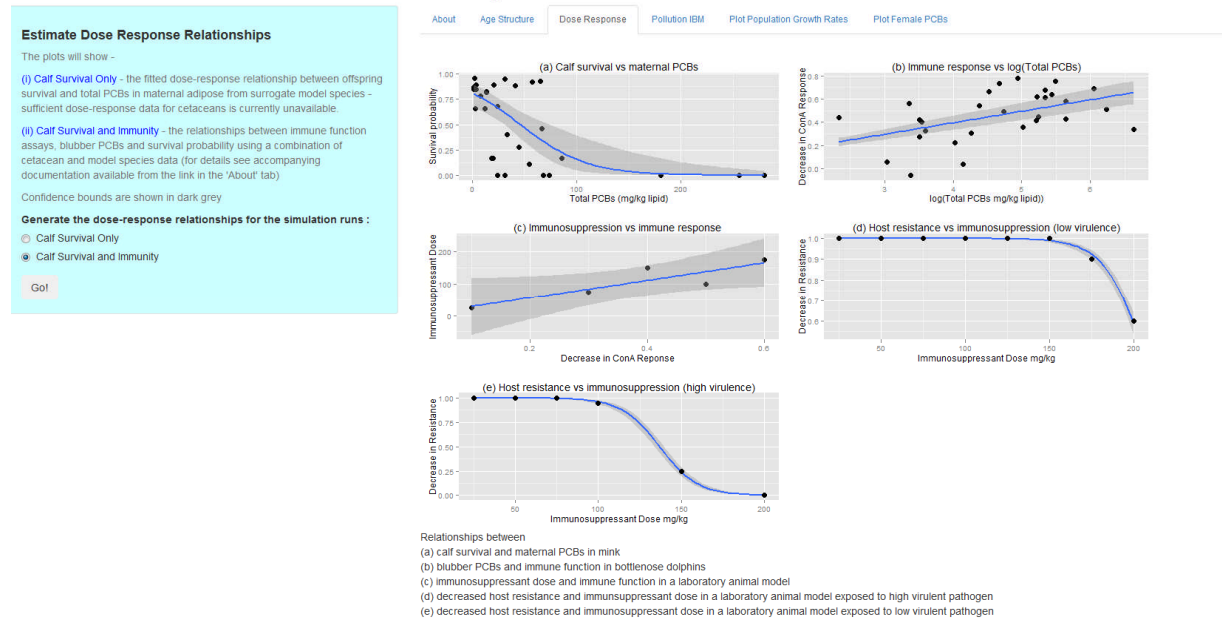
Figure 3. The dose response tab with the ‘calf survival only’ option chosen by the user displays the relationship used to modify calf survival based on maternal PCB blubber concentrations.

(ii) Effects of PCBs on calf survival and immunity (Fig. 4.). By clicking on the ‘calf survival and immunity’ radio button the user can choose to use a combination of modified calf survival and additionally investigate the effects of PCBs on immunity to estimate how that may affect survival following exposure to a pathogen. This is then requires three modelling stages:-

1. Use the relationship between blubber PCBs and the proportional decrease in an *in vitro* immune response measure known as ConA [for details of this measure, see Schwacke et al. (2012)] to estimate the change in immune response for a given concentration of blubber PCB.
2. Use the relationship between the proportional decrease in ConA response and the degree of whole animal immunosuppression to which that measure relates (as determined in the US National Toxicology Program (NTP) studies in mice, reported by Luster et al. (1993)). This is given in term of the dose of an immunosuppressant compound (cyclophosphamide) that was administered to the animals.
3. Finally use the relationship between the dose of immunosuppressant and the decrease in host resistance following exposure to a pathogen, either of low or higher virulence again as reported by Luster et al (1993) from the NTP studies. This gives a multiplier which is used to modify the probability of survival – so a factor of 1 would not change the background survival probability even after exposure to a pathogen but a factor of 0.5 would result in a halving of the survival probability.

In this way the concentration of PCBs in the blubber can be related to changes in host resistance and the impact that may have on survival can be investigated in the overall population through its ultimate effect on potential

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population growth.

Figure 4. The dose-response tab with the 'calf survival and immunity' option chosen shows the relationships between PCBs and offspring survival (a) and between PCBs and immunosuppression (b-e).

Pollution IBM Tab

This user interface sets the final parameters for the individual based model and generates the population trajectories for 100 years for the number of simulations specified (Fig. 5). In the first input box the user can indicate the number of simulations. The models take quite a bit of time to run so it would be recommended that the user carries out a few simulations (<10) to see how the population trajectories might look before carrying out a larger number.

The first slider lets the user choose the annual accumulation of PCBs in the individual animals.

The second and third sliders let the user determine the proportion of the female PCBs that are transferred to the offspring during lactation and *in utero*.

In the next section the user can specify if they would like to generate a set of simulations where the concentration of PCBs declines over time (as recommended by the Pollution 2020 Steering Group). This may be useful where the starting population is based on historic data when the levels of PCBs in the environment were much higher than the contemporary levels. The simulations will run using the annual accumulation as chosen in the first slider and then will decrease the annual accumulation by the specified proportion (i.e. 0.01 would be an annual decrease of 1%). Setting this to zero will run the simulations with no change in accumulation concentrations over time.

Finally this tab allows the user to choose which of the dose-response functions to include, what proportion of the population is exposed to a pathogen if immune effects are of interest and whether that pathogen is low or high virulence.

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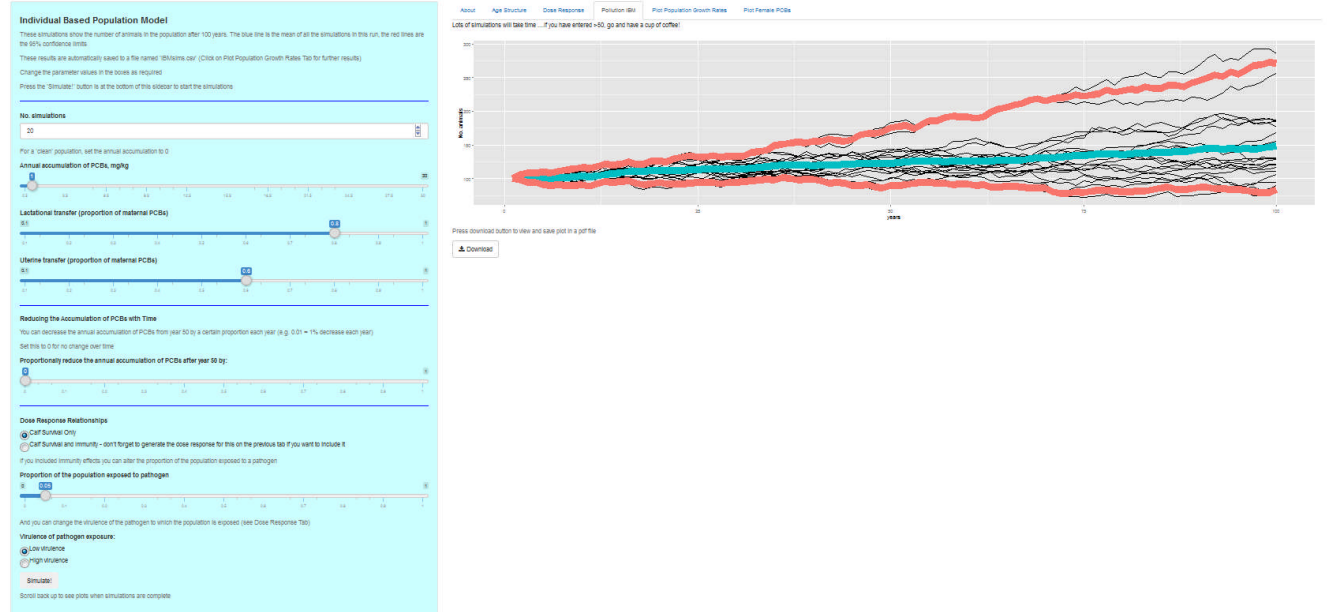


Figure 5. The Pollution IBM tab displays the user interface to select the final input parameters for the individual based population simulations and generates a plot to show the population trajectories for the chosen number of simulations (in this case 20 simulations).

Plot Population Growth Rates Tab

In this tab the user can then upload the most recent set of simulations for further visualisation and analysis. The histogram shows the frequency distribution of all the simulations in the set (the 20 simulations from Fig. 5 are displayed in the screen shot in Fig. 6). This shows the degree of uncertainty in the change in potential population growth. It also reminds the user of the annual accumulation rate and whether any proportional decline in PCBs was included. The mean population growth rate and the 95% confidence intervals calculated from the population growth trajectories between years 60 and 95 of the 100 years are given. These can then be compared between different exposure and population scenarios by downloading the results into a csv file.

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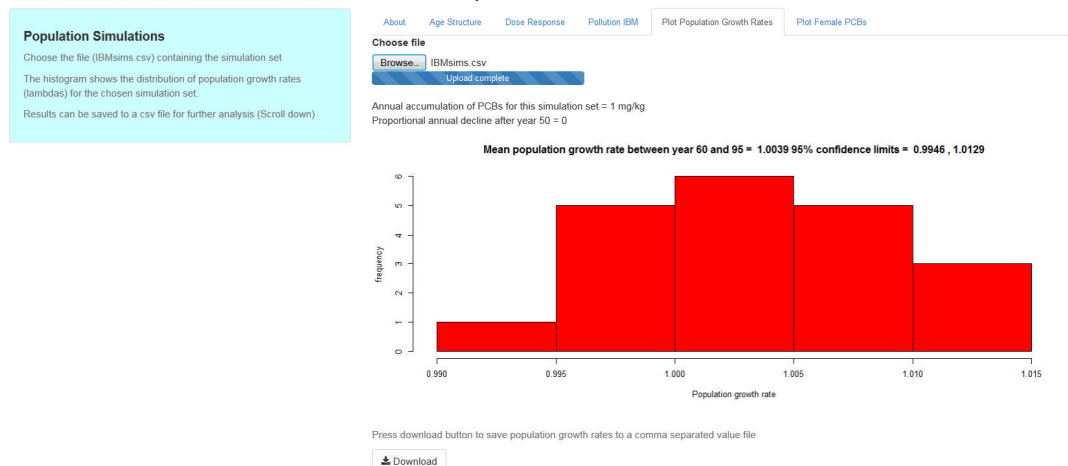


Figure 6. The user can then upload the data from the previous simulation set to see the range of population growth rates generated by the stochastic individual based model.

Plot Female PCBs Tab

The final tab allows the user to plot the concentration of PCBs in the females by age generated by the preceding set of simulations. The mean for each age class is shown (red line in the Fig. 7) and shows the mean concentration in the all the adult females between the age of sexual maturity and the maximum age as set by the user in the first tab. The plots and data can be saved and can be compared to any available empirical data to see how the model outputs compare with which is known about the particular species and population of interest.

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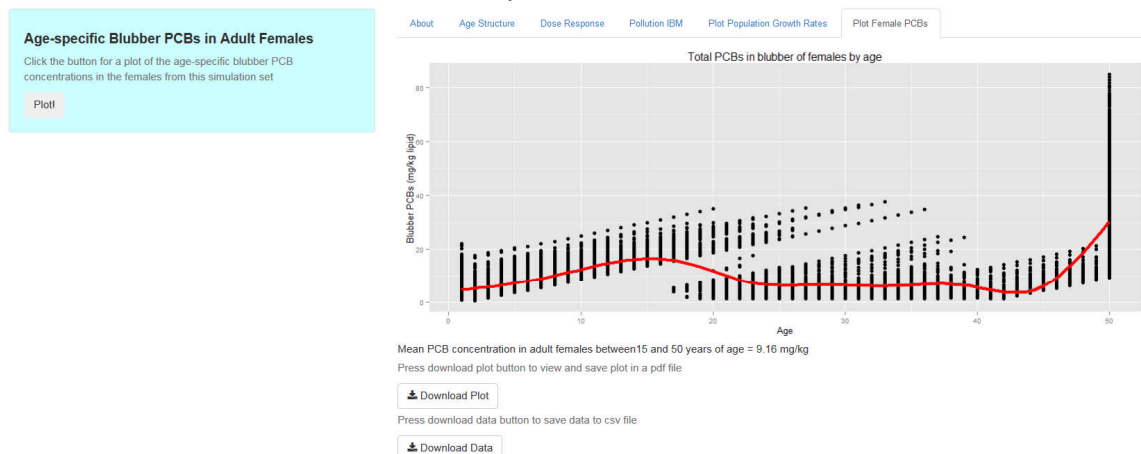


Figure 7. The final tab plot showing the age-specific estimated concentration of PCBs in the adult females from the preceding set of simulations.

Conclusion

Once any final errors have been rectified or minor modifications have been completed, this application will be made available to the wider research community and will initially be hosted on a server at the Sea Mammal Research Unit at the University of St Andrews. The code will also be made available on GitHub (<https://github.com/>) a hosting website for code review and management for open source software. This will allow users to access the full code, both the R Program code (a program for statistical computing, <http://www.r-project.org/>) and the user interface which used a package called Shiny, freely available from R-Studio (<http://www.rstudio.com/>).

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