(1) This "readme" file accompanies software (Windows-based PCs) for the July 2011 version of the Agency's methodology for assessing impacts of atrazine on aquatic plant communities. This software consists of:

(a) Fortran code and executable files for the program "AtrazineLOCPATICalculation", and input files for this program in a zip file.

(b) Fortran code and executable files for the program "AtrazineChemographAnalysis".

(2) The executable programs provided here do not require an installation routine. They simply need to be copied to a desired directory and run. Each executable runs in a DOS-window, so that user interaction is on a line input/output basis, not with a visual interface. The FORTRAN code is provided for review purposes, but, if used to generate new executables, it was developed using Intel Visual Fortran Version 9.1 under Microsoft Visual Studio 2005, and uses utilities from the IMSL mathematical library provided with Visual Fortran.

(3) The risk assessment methodology embodied in this software is described in other posted documents, especially the report *Proposed Methodology for Specifying Atrazine Levels of Concern for Protection of Plant Communities in Freshwater Ecosystems* (Erickson 2010) and a 2011 addendum to this report. Briefly, this methodology is a follows:

(a) Information from single-species aquatic plant toxicity tests with atrazine is used to compute daily "Plant Assemblage Toxicity Index" (PATI) values for exposures of interest, these daily PATI values being the average reductions in growth rate across a specified assemblage of plant species at each day's concentration.

(b) The daily PATI values are summed to provide a cumulative PATI value that represents the total severity of toxicity in an exposure of interest. If the exposure is longer than 60 days, this summation is limited to the contiguous 60 days resulting in the highest cumulative PATI value. The use of a cumulative PATI with a 60 day assessment period deviates from Erickson (2010) as explained in the 2011 addendum to this report.

(c) The relationship of effects of atrazine on aquatic plant communities in experimental ecosystem (microcosm/mesocosm or "cosm") exposures to the cumulative PATI values for these exposures is evaluated to determine what value for the cumulative PATI is a level of concern (LOC_{PATI}) – based on effects in the experimental systems.

(d) Cumulative PATI values are calculated for field exposure time series to determine whether and by how much these exposures exceed the LOC_{PATI}.

(e) An LOC based directly on exposure concentrations (rather than PATI) can be developed using the relationship between average concentrations and cumulative PATI values in typical field exposures. Such an LOC is not an aspect of the software being provided here, but is discussed elsewhere on the website.

(4) The first program, AtrazineLOCPATICalculation_July2011, calculates LOC_{PATI} based on the set of experimental ecosystem studies with atrazine described in the memorandum *Bibliography of Microcosm and Mesocosm Studies and Criteria Used to Screen Studies for Analysis of Atrazine Risks to Aquatic Plant Communities* posted on this website. PATI values for the cosm exposures are based on the overall distributions of toxicity test parameters reported in Erickson (2010). The toxicity distributions are incorporated into the code, while the cosm data are in the provided zip file. This program will:

(a) Cue the user for an assessment period (in days), the current choice for this in the Agency's methodology being 60. This input option was provided for development purposes.

(b) Cue the user for a file containing the cosm effects data. The file provided in the zip file is "CosmEffects.dat", which reflects the above-cited memorandum. This is an ASCII file with one line for each cosm exposure consisting of (i) a three character field containing an alphanumeric identification code (left justified if less than 3 characters) for the exposure, (ii) a five character field containing an integer (right justified) designating the exposure duration in days, and (iii) a three character field containing an integer (right justified) set to 1 if there was a significant adverse effect and 0 otherwise. In addition, for each cosm exposure, there is a separate file containing a concentration time series for that exposure. Each file is named "Exposure#AAA.txt", where AAA is the alphanumeric identification code, right truncated if the code is less than three characters. These files must be in the same directory from which the program is executed.

(c) Cue the user for the name of an output file. The program will then input the cosm data, compute the cumulative PATI for each cosm exposure, conduct a binary logistic regression of cosm effects versus PATI to determine an LOC_{PATI}, and prepare the output file. The output file will provide the cumulative PATI value for each cosm exposure, information on the regression results, and the final LOC_{PATI} value.

(5) The second program, AtrazineChemographAnalyses_July2011, uses the above LOC_{PATI} to evaluate user-provided exposure time series (chemographs). Using the same toxicity test parameters as the LOC program, it will calculate the cumulative PATI for each chemograph and calculate the ratio of this to LOC_{PATI}, this ratio being termed the "effects exceedence factor" (EEF). It will also compute the maximum running average concentration for each chemograph using a user-specified averaging period, a calculation which was provided to support development of concentration-based LOCs. The steps in this program are:

(a) Cue the user for the LOC_{PATI} determined in the LOC program.

(b) Cue the user for the assessment period of PATI. This must match what was used to calculate the LOC_{PATI}.

(c) Cue the user for the averaging period to derive the maximum running average concentrations. This need not be the same as the PATI assessment period

(d) Cue the user for the name of an ASCII file consisting of names of files containing the concentration time-series for each chemograph. The first line of this file is an integer designating the number of chemographs to be assessed. Each subsequent line is the name of a concentration time-series file for a particular cosm exposure. If the complete directory path is not given for this file, the file must be in the directory from which the program is being executed. Each of concentration time-series files consists of 365 lines, each line consisting of the Julian day (integer) and the concentration (ug/L) on that day (integer or decimal number). The numbers can be separated by either spaces or a comma.

(e) Cue the user for the desired name for the output file. The program will then input the chemograph data, calculate the cumulative PATI for each chemograph using the same toxicity distributions as in the LOC program, calculate the EEFs and the running average concentrations, and prepare the output file. The output file consists of one line confirming the LOC_{PATI} and the assessment period, and then a table showing each chemograph file name with its running average concentration, its cumulative PATI value, and its EEF.