# Interim Guidance for Using Ready and Inherent Biodegradability Tests to Derive Input Data for Multimedia Models and Wastewater Treatment Plants (WWT) Models (9/1/2000)

Multimedia fate models such as the EQC and wastewater treatment plant models (e.g. STP, ASTREAT) require transformation half-lives for the appropriate compartments. In the case of EQC and similar box models which include atmospheric, aquatic and terrestrial fate processes in a defined environment, bulk compartmental half-lives are required for air, water, soil and sediment. WWT Models that describe typical sewage treatment operations similarly require half-lives for the compartments in which transformation may occur. For WWT models these may include primary treatment (gravitational settling of influent sewage), activated sludge secondary treatment, and secondary sludge settling. For all of the compartments listed above except the air compartment in EQC, biodegradation is often the most important process determining the fate of the compound of interest. Unfortunately, measured values for these half-lives are often unavailable, and this means that other ways must be found to obtain the needed model inputs.

EPA has developed interim methods for deriving these data from Ready and/or Inherent Biodegradability test data. EPA has received numerous requests for this interim guidance and is therefore making it available in the hopes that experienced scientists will find it helpful and will contribute to the further development and validation of these methods. These methods should be regarded as interim guidance, and used only with appropriate attention to their intended application as well as scientific uncertainties. The intended applications are limited screening-level determinations of environmental transport and transformation using multimedia or Mackay-type box models; they do not include quantitative exposure or risk assessment. Further, even though these methods do use measured biodegradability data as the starting point, Ready and Inherent tests are by nature far removed from environmental conditions. Their purpose is not simulation but rather simply to indicate whether a substance is easily biodegradable or not. Therefore, estimated half-lives derived using this methodology should never be used when reliable measured biodegradation half-lives are available. EPA will continue to further refine and validate these methods and will update this interim guidance as appropriate

Finally, the user must understand that there remain substantial scientific uncertainties in the suggested estimation methods. Some validation work has been performed but is not yet published (reference 1). Overall, the results neither bolster nor contradict the interim methods, and mostly illustrate the shortage of high quality half-life data. This means that the methods remain largely unvalidated. Among the assumptions is that intermediate results from a Ready or Inherent test can be used to derive intermediate half-lives. It is unclear that this is reasonable given that these test methods tend to give all or nothingresults and are normally regarded as pass/fail tests. And even if it turns out that Ready and Inherent test data can be used to assign half-lives as proposed, the specific numbers suggested as cut-points (e.g., 20% and 40% of theoretical ultimate degradation in the Ready test) were selected based on judgment and may not be the best for present purposes.

Another key assumption is that in the absence of test data, it is acceptable to use simple multipliers to relate half-lives for water, soil and sediment; for example, to estimate soil and sediment half-lives from a water half-life. Some validation of this approach has been published (see references 2 and 3), but much more is needed. Last, the user should keep in mind that in the environment a wide range of half-lives is likely to be a much more realistic depiction of environmental fate; but for each run of a model like EQC a single value must be selected for a given compartment. This is highly unrealistic. Ideally, half-lives should be expressed as ranges, and multimedia model results (e.g., overall persistence) should be given as distributions, not single values (reference 4).

**References**

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2. Boethling RS, PH Howard, JA Beauman and ME Larosche. 1995. Factors for intermedia extrapolation in biodegradability assessment. Chemosphere 30: 741-752.

3. Federle TW, SD Gasior and BA Nuck. 1997. Extrapolating mineralization rates from the ready CO2 screening test to activated sludge, river water and soil. Environ. Toxicol. Chem. 16: 127-134.

4. Webster E, D Mackay and F Wania. 1998. Evaluating environmental persistence. Environ. Toxicol. Chem. 17: 2148-2158.

**Methods To Input Data**

- Using Ready and Inherent Biodegradability Data to Derive Input Data for WWT Models
- Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model

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**Using Ready and Inherent Biodegradability Data to Derive Input Data for WWT Models**

The scheme in Table I is offered as an interim procedure for assigning activated sludge half-lives for input to models of activated sludge (AS)-based wastewater treatment (WWT) plants:

**Table I Proposed Scheme**

| Ready test result | Inherent test result | Activated sludge half-life, hr |
|---|---|---|
| pass test | -- | 1 |
| no pass, but >= 40 % | -- | 3 |
| no pass: >= 20 but < 40 % | >= 70 % | 10 |
| -- | >=20 but < 70 % | 30 |
| no pass: < 20 % | < 20 % | 10,000, or current default for no biodeg if different |

The suggested AS half-lives of 1, 3, 10 and 30 hr are from Mackay's guidance for the STP model, and correspond to their designations of rapidly, moderately, slowly but significantly, and very slowly biodegradable, respectively. Some rules are needed for what to do when there are both ready and inherent biodegradability test data, especially when there are apparent conflicts. The following are suggested: (1) ready test results >= 40 % take precedence over inherent results regardless of what they are; (2) inherent test results take precedence over ready test results if the latter are < 40 %.

If the STP model is run for a hypothetical chemical that has water solubility = 10E+06 mg/L; log Kow = -2; v.p. = 10E-06 Pa; MW = 180 (roughly the properties of glucose, a rapidly biodegradable, water soluble, nonvolatile, non-adsorbing chemical), removal estimates are as follows for the activated sludge half-lives given above: 94; 80; 47; 23 %. (It is assumed for this exercise that the half-lives for the aeration basin and secondary settling chamber are equal, but the half-life for the primary clarifier is 4x greater, as recommended by Mackay).

It is of interest to compare this to the guidance in the EU Technical Guidance Document (TGD). Table II presents an interpretation of the TGD guidance relative to interpretation of ready and inherent test data:

**Table II TGD Scheme**

| Ready test result | Inherent test result | Activated sludge half-life |
|---|---|---|
| pass test, including 10-day window | -- | 0.69 hr (k = 1.0 hr-1) |
| meet final pass criterion but not 10-day window | -- | 2.3 hr (k = 0.3 hr-1) |
| fail both criteria | -- | (k = 0) |
| -- | >= 70 % | 6.9 hr (k = 0.1 hr-1) |
| -- | < 70 % | (k = 0) |

Comments and interpretation

In the TGD scheme (Table II), if a chemical meets the final pass criterion (this means either > 60 % ThOD; or > 60 % TCO2; or > 70 % DOC loss) as well as the 10-day windowcriterion in the normally stringent ready test, it is assigned an AS t1/2 of 0.69 hr (rate constant of 1 hr-1). If it meets the final pass criterion but not the 10-day window, it may be assigned a slightly lower rate constant (equivalent to a half-life of 2.3 hr). If it does not pass--e.g. even if it just misses the final pass criterion--it is assigned no biodegradation in treatment (rate constant of zero, for which the half-life is infinite)....unless it is tested in an inherent test and meets the >= 70 % DOC loss criterion. In this case it is assigned a rate constant of 0.1 hr-1 (half life of 6.9 hr), which corresponds roughly to the Mackay designation slowly but significantly biodegradable. If the inherent test result misses the 70 % mark, the assigned sludge half-life again is infinite.

Assuming no biodegradation for chemicals that just miss the final pass criteria does not seem reasonable and the scheme in Table I, in contrast, is designed to give credit for degradation that is certainly significant, while missing the formal pass criteria. Degradation of 45, 50, 55 % of theoretical is often observed in ready tests and probably represents nearly complete ultimate biodegradation in most cases. Since ready tests are stringent, this should correspond to very significant removal in treatment. The Mackay term moderately degradableapplies and the assumed AS half-life is 3 hr. If the ready test result is in the 20-40 % range, given the stringency of ready tests this is still significant, but obviously should be assigned a higher sludge half-life (Table I assigns 10 hr). If the ready result is < 20 %, it is appropriate to consider the AS rate constant to be zero, but not if there is an inherent biodegradation test result (usually this would be the Zahn-Wellens/EMPA test; OPPTS 835.3200) showing significant (defined as > 20 % DOC loss) degradation. In this case an AS half-life of either 10 hr (if the Z-W result is > 70 %), corresponding to the Mackay designation slowly but significantly biodegradable, or 30 hr (if the Z-W result is in the 20-70 % range), corresponding to the Mackay designation very slowly biodegradable, is assigned. If the inherent result is < 20 %, it is appropriate to assume degradation in sludge is negligibly slow (STP default half-life of 10,000 hr).

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**Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model**

Multimedia fate models like the EQC model require compartmental half-lives for air, water, soil and sediment. The scheme in Table I is offered as an interim procedure for assigning half-lives for input to such models. These are bulk half-lives; i.e., for the compartment as a whole. They are not to be interpreted as (necessarily) half-lives for any specific process such as biodegradation. No assumptions should be made that compromise their interpretation as bulk half-lives, such as that biodegradation is the important process and occurs in soil pore water only. Air half-lives are not addressed here and it is assumed that data for input to models are either measured or derived from the Atmospheric Oxidation Program (AOP) or similar methodology.

**Table I** **Proposed Scheme**

| Ready test result | Inherent test result | Water half-life, d | Rate constant |
|---|---|---|---|
| pass test | -- | 5 | 0.14 d-1 |
| no pass, but >= 40 % | -- | 10 | 0.069 d-1 |
| no pass: >= 20 but < 40 % | >= 70 % | 30 | 0.023 d-1 |
| -- | >=20 but < 70 % | 100 | 0.0069 d-1 |
| no pass: < 20 % | < 20 % | 10,000, or other | (k = 0) |

default for no
biodeg as appropriate

Some rules are needed for what to do when there are both ready and inherent biodegradability test data, especially when there are apparent conflicts. The following rules are suggested: (1) ready test results >= 40 % take precedence over inherent results regardless of what they are; (2) inherent test results take precedence over ready test results if the latter are < 40 %. Half-lives for the soil compartment are assumed to be the same unless compelling evidence to the contrary is available. This must consist of experimental data specific for the given substance. Half-lives for the sediment compartment are assumed to be 3-4 times longer than for water and soil, unless, again, there is convincing experimental evidence to the contrary. These assumptions are discussed in more detail below.

Table II presents a reasonable interpretation of the EEC Technical Guidance Document (TGD; EEC 1996) relative to extrapolation of ready and inherent test data to surface waters, and is provided for comparison to the scheme in Table I. The TGD does not give default (bulk) compartmental half-lives for soil and sediment, but rather presents a methodology for assigning half-lives based on ready or inherent biodegradability test data and additional information on the solids/water partition coefficient for the chemical. This parameter can be calculated from other data such as Kow after making certain assumptions.

**Table II TGD Scheme**

| Ready test result | Inherent test result | Surface water half-life | Rate constant |
|---|---|---|---|
| pass test, including 10-day window | -- | 15 d | k = 0.047 d-1 |
| meet final pass criterion but not 10-day window | -- | 50 d | k = 0.014 d-1 |
| fail both criteria | -- | infinite | k = 0 |
| -- | >= 70 % | 150 d | k = 0.0047 d-1 |
| -- | < 70 % | infinite | k = 0 |

Comments and interpretation

In the TGD scheme (Table II), if a chemical meets the final pass criterion (this means either > 60 % ThOD; or > 60 % TCO2; or > 70 % DOC loss) as well as the 10-day windowcriterion in the normally stringent ready test, it is assigned a water half-life of 15 days. If it meets the final pass criterion but not the 10-day window, it is assigned a lower half-life of 50 d. If it does not pass--e.g. even if it just misses the final pass criterion--it is assigned no biodegradation in surface water (rate constant of zero, for which the half-life is infinite)....unless it is tested in an inherent test and meets the >= 70 % DOC loss criterion. In this case it is assigned a half life of 150 d. If the inherent test result misses the

70 % mark, the assigned half-life again is infinite. Giving some credit for less-than-perfect results (meeting the ready biodeg final pass criterion but failing the 10-day window)--namely, assigning a rate constant of 50 rather than 0 days as might have been done (Table II)--is a step in the right direction. However, the 10-day window may no longer be widely enforced in Europe and Painter (1995) has recommended that it be discarded. Federle et al. (1997) also questioned the validity of the concept. Further, given the stringency of ready tests, assuming no biodegradation for chemicals that just miss the final pass criteria does not seem reasonable--i.e. is excessively conservative.

The starting point for developing the scheme in Table I is the assumption that chemicals that meet the final pass criteria for ready biodegradability tests do so because they have been completely biodegraded by the end of the test, which normally occurs at 28 days. Although the precise definition of completely degradeis somewhat arbitrary, 5-6 half-lives will lead to 97-98 % loss of parent material and if the test period is 28 days, this implies a half-life no greater than about 5 days assuming first-order kinetics. Struijs and van den Berg (1995), whose work formed the basis of the TGD guidance, came to roughly the same conclusion though they did not explicitly recommend this half-life as the default for chemicals passing a ready test.

The scheme in Table I is also designed to give credit for degradation that is certainly significant, despite missing the formal pass criteria. The rationale is that degradation of 45, 50, 55 % of theoretical is often observed in ready tests and probably represents nearly complete ultimate biodegradation in most cases. Since ready tests are stringent, this should correspond to a very significant biodegradation rate in surface waters: Table I assigns a half-life of 10 days. If the ready test result is in the 20-40 % range, given the stringency of ready tests this again should be viewed as significant, but the substance should be assigned a higher half-life (Table I assigns 30 days). If the ready result is < 20 % it is appropriate to consider the rate constant to be zero, but not if there is an inherent biodegradation test result (usually this would be the Zahn-Wellens/EMPA test; OPPTS 835.3200) showing significant (defined as > 20 % DOC loss) degradation. In this case a half-life of either 30 days (if the Z-W result is > 70 %) or 100 days (if the Z-W result is in the 20-70 % range) is assigned. If the inherent result is < 20 %, it is appropriate to assume degradation in surface water is negligibly slow. The 10-day window concept is not employed in this scheme.

Extrapolation to soil and sediment

As stated above, Struijs and van den Berg (1995) developed guidance for extrapolating results of standard OECD biodegradation test methods to various environmental conditions. The extrapolation protocol is based on generic microbial population densities, which are assumed to be 100 times higher for soil pore water than for surface water. Equilibrium partitioning (which requires additional information on solids/water distribution) is then used to adjust the predicted biodegradation rate for distribution of the chemical between sediment and pore water (i.e., for sorption), and it is assumed that no degradation occurs in the bound phase. The authors state that the protocol yields reasonable predictions of soil biodegradation rates from ready biodegradability test results, but the number of chemicals studied was small. More importantly, this approach requires assumptions about bioavailability that are open to question, and in any case are unnecessary when the only parameters needed from this exercise are bulk compartment half-lives for input to a multimedia fate model.

Another approach to getting the required soil and sediment half-lives is to use the recommended values for water and extrapolate to the other media using scaling factors. Scaling factors are numbers which, when multiplied by a degradation rate constant or half-life for one set of environmental or test conditions, yield a rate for a second, different set of conditions.

Boethling et al. (1995) collected measured half-life data for a wide variety of chemicals that had been tested in both soil and water samples collected from the environment. They then calculated mean ratios of half-life in water to half-life in aerobic surface soil for 20 chemicals. The ratios varied widely but the overall mean was around one, suggesting that for screening purposes, it is valid to assume that biodegradation in aerobic surface waters is about as fast as degradation in aerobic surface soil. Boethling et al. (1995) also compared biodegradation in aerobic surface soil to anaerobic degradation in flooded soil, and they found that for chemicals without nitro groups (which are rapidly reduced anaerobically), aerobic degradation was on average 3-4 times faster than anaerobic degradation. Again, the actual ratios of mean half-lives varied widely for the chemicals studied.

Federle et al. (1997) compared degradation rates under various conditions in much the same fashion as in Boethling et al. (1995), but the experimental data were generated de novo under carefully controlled conditions, as opposed to being gathered from the literature. Scaling factors for river water vs. soil varied widely as was observed in the earlier study, but the overall mean was close to one as in Boethling et al. (1995). Federle et al. (1997) did not include sediment in their study. They also found that, contrary to the results of Struijs and van den Berg (1995), biodegradation rates in river water vs. soil were not proportional to microbial density, even if the different biodegradabilities of sorbed vs. free chemical were factored into the comparison.

These studies suggest that half-lives in bulk soil may be assumed for screening purposes to be about the same as for surface water, and that sediment half-lives may be assumed to be 3-4 times longer.

References

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