Climate Variability and Change—Hydrological Impacts (Proceedings of the Fifth FRIEND World Conference held at Havana, Cuba, November 2006), IAHS Publ. 308, 2006.

A global assessment of chemical effluent dilution capacities from a macro-scale hydrological model

VIRGINIE D. J. KELLER[1], MICK J. WHELAN[2] & H. GWYN REES[1]

1 *Centre for Ecology and Hydrology, Wallingford, Oxfordshire OX10 8BB, UK*
vke@ceh.ac.uk

2 *Safety and Environmental Assurance Centre, Unilever Colworth, Colworth Park, Bedfordshire MK44 1LQ, UK*

Abstract Environmental risk assessments for "down-the-drain" chemicals (e.g. pharmaceuticals and household product ingredients) are generally based on a comparison between predicted environmental concentration (*PEC*) and predicted no effect concentrations (*PNEC*) for a generic environment with a fixed dilution factor. For PEC calculations spatial and temporal variability is often not explicitly taken into account. In the absence of detailed local-scale information for specific point-sources, spatially-explicit approximations can be made, based on the ratio of available surface water and domestic water consumption. In this paper, a new methodology is proposed for predicting surface water dilution at a global scale. The approach employs 0.5° resolution geographical data on national boundaries, population density, runoff (from water balance model calculations) and domestic water consumption to produce dilution factor maps for the global land surface. The proposed methodology has great potential for improving screening-level chemical risk assessments.

Key words chemicals; dilution; environmental risk assessment; GIS; global-scale; population; runoff

INTRODUCTION

Environmental risk assessments for chemicals usually make comparisons between Predicted Environmental Concentrations (PECs) and Predicted No Effect Concentrations (PNECs). For many so-called "down-the-drain" chemicals (such as pharmaceuticals and the ingredients used in household cleaning products), the principal disposal route after use is via the wastewater stream. Screening-level exposure assessments (i.e. PEC calculations) for these substances are usually based on a simple ratio of per capita chemical consumption and per-capita domestic water use. This is then adjusted for removal during sewage treatment, if applicable, and for dilution in the receiving aquatic environment using a generic dilution factor (e.g. EC, 2003). This approach is simple but it is also reasonably robust scientifically and is appropriate for comparative screening-level risk assessments. However, it does not take into account spatial and temporal variability in dilution which changes with the relative magnitude of point-source loads and river discharge at the point of emission. This information may be required when trying to compare risks in different geographical areas with different hydrological regimes and population densities. In the absence of detailed local-scale information for specific point-sources, tolerable spatially-explicit approximations can be made, based on the ratio of available surface water and domestic water consumption, for discrete areas. Reasonable estimates of mean monthly and mean annual runoff can be obtained from long-term meteorological data using simple water balance models. Domestic water consumption can be estimated from country- or region-specific data for per-capita domestic water use and population density. These calculations allow the spatial variability of dilution and its seasonality to be examined at different spatial scales (catchment, regional, national and continental) anywhere in the world.

This paper presents a new methodology which has been developed to estimate the spatial variability of dilution factors using global-scale data. These predictions will inevitably be crude estimates of local conditions which will vary on a case by case basis but may provide a reasonable initial estimate which can be refined locally if required (e.g. using more sophisticated exposure assessment tools such as GREAT-ER (Feijtel *et al.*, 1997). The approach can be used to compare screening-level *PEC*s on a regional, country-specific or catchment basis and help to identify geographical areas with relatively high risk ("hot spots"), thereby guiding targeted risk mitigation measures at various scales. It can also be used to help generate statistical distributions of *PEC* required in probabilistic risk assessments.

APPROACH

The methodology was specifically derived for estimating concentrations of "down-the-drain" chemicals in fresh surface waters.

Concept

PEC for raw waste water (PEC_{SEWAGE}) can be estimated from:

$$PEC_{SEWAGE} = \frac{U}{W} \tag{1}$$

where U is the daily per capita consumption of chemical (mg cap^{-1} day^{-1}) and W is the daily per capita water use (L cap^{-1} day^{-1}). U is calculated from the annual mass of chemical used nationally, T (t year^{-1}) using:

$$U = \frac{T \cdot 10^9}{365 \cdot P_{COUNTRY}} \tag{2}$$

where $P_{COUNTRY}$ is the population of the country concerned. The surface water PEC (PEC_{AQ}), immediately after mixing, but before any decrease in chemical concentration has occurred as a consequence of degradation and dilution, can be estimated from:

$$PEC_{AQ} = \frac{(1-F) \cdot PEC_{SEWAGE}}{DF} \tag{3}$$

where F is the fraction of chemical removed in wastewater treatment, derived from monitoring data or from standard laboratory biodegradation and partitioning studies. DF is the dilution factor which is defined as:

$$DF = \frac{(Q+q)}{q} \tag{4}$$

where Q is the discharge (m^3 s^{-1}) of the receiving water and q is the point-source discharge (m^3 s^{-1}). Unfortunately, in many parts of the world, the data required to estimate DF at a local (catchment or river reach) scale is not readily available. However, a proxy for DF can be derived from public-domain gridded runoff R (mm year^{-1}) and population density ρ (cap m^{-2}) data sets which are available at a global scale. Using gridded data and adopting dimensional units, DF, for any grid cell at a specified resolution can be defined as:

$$DF = \frac{Q_i + q_i}{q_i} = \frac{\sum_{j=1}^{i}(R_j \cdot A_j) + W_i \cdot A_i \cdot \rho_i}{W_i \cdot A_i \cdot \rho_i} \tag{5}$$

where W is the domestic water use per capita (L^3 cap^{-1} T^{-1}), A is the cell area (L^2), i is an index for any cell in the grid and j is an index for all cells contributing flows to cell i (i.e. defined by cell-to-cell flow routing from the topographic divide).

Runoff data

Long-term average (usually 1960–1990) annual runoff can be predicted using macroscale hydrological models (e.g. Arnell, 1999). Such models, which commonly have a resolution of 0.5º latitude by 0.5º longitude, have been used to define land-surface parameterization schemes in general circulation models (e.g. Nijssen *et al.*, 1997) and for estimating water resource availability at global, continental or regional scales (e.g. Alcamo *et al.*, 2003; Abdulla & Lettenmaier, 1997).

In this paper, the composite runoff fields produced by Fekete *et al.* (1999) were used. These runoff estimates were generated by combining a simple water balance model with observed river discharge data. The water balance model uses the data set of Legates & Willmott (1990) for global precipitation, soil type data from the FAO/UNESCO soil data bank (FAO/UNESCO, 1986), topographic data from the ETOPO5 global elevation data set (Edwards, 1989) and a contemporary

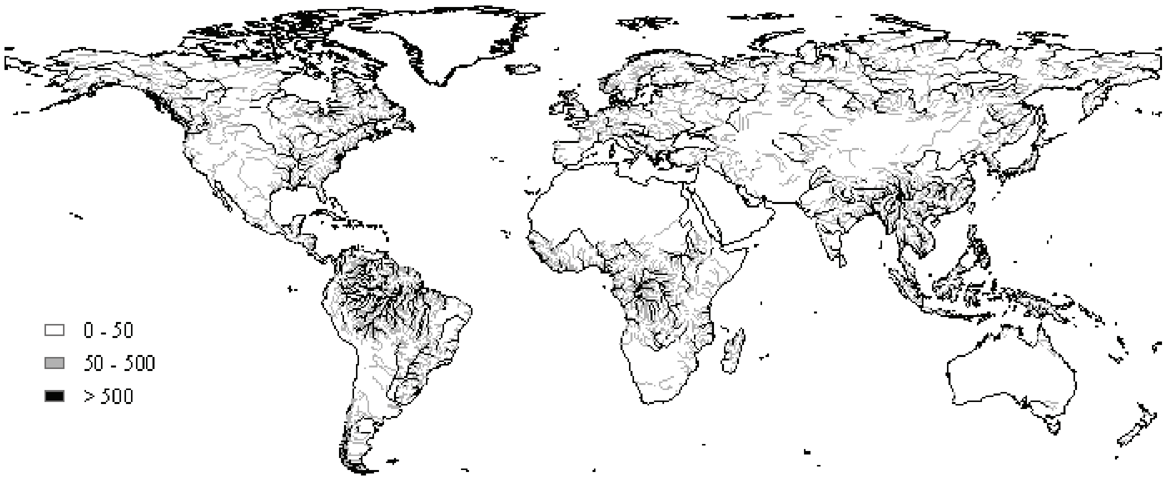

Fig. 1 Predicted river discharge ($m^3 s^{-1}$) from the annual composite runoff fields (CRF) data (Fekete *et al.*, 1999).

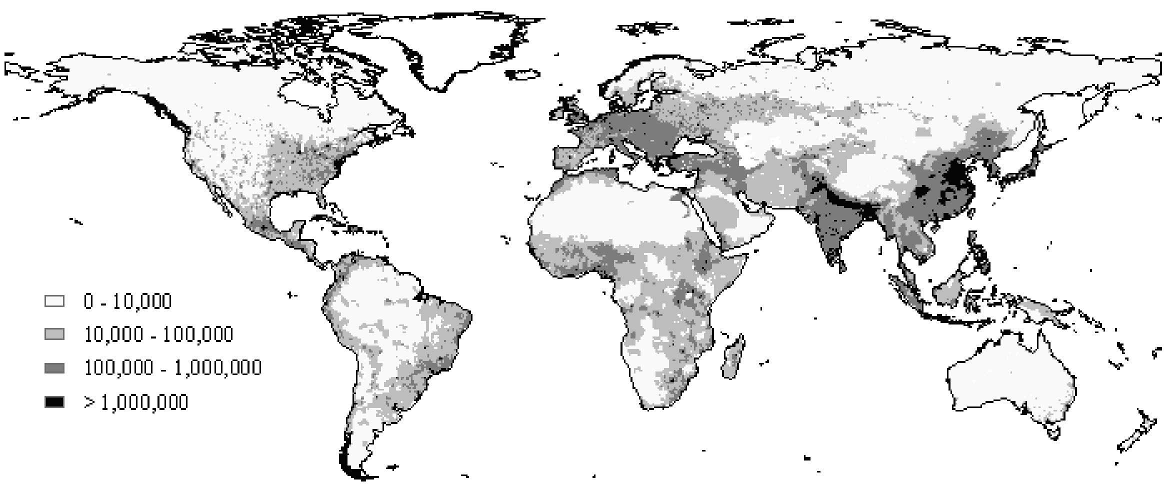

Fig. 2 Global population per grid cell derived from the Gridded Population of the World (GPW) v.2 data set for 1995 (SEDAC, 2000), degraded to 0.5° × 0.5° resolution.

land cover classification derived from the Terrestrial Ecosystem Model (Melillo *et al.*, 1993) and Olson's land use classification (Olson, 1992).

The topographically-derived flow direction grid provided by Fekete *et al.* (1999) was used for accumulating runoff in the grid, thereby estimating cell-specific discharge Q_i (Fig. 1).

Population data

The GPW v.2 data set for 1995 (Gridded Population of the World – GPW, SEDAC, 2000) was used to estimate the distribution of global population density. This data set has been adjusted to correspond with national-level population estimates issued by the United Nations. The resolution of the original data was 2.5 arc minutes which was aggregated to a 0.5° ×0.5° (latitude, longitude) resolution corresponding to the runoff grids (Fig. 2).

Domestic water use

Per-capita domestic water use (W) varies widely from country to country and even within countries as a consequence of water availability, infrastructure, wealth and habits. Individual values of W were generated for each 0.5° × 0.5° grid cell using mean values for each country. National statistics were extracted from several public domain data sources (Gleick, 1996; OECD, 2002; WRI, 2003, FAO, 2000). Where discrepancy existed between data sources, the lowest value was selected to provide a more conservative value for DF.

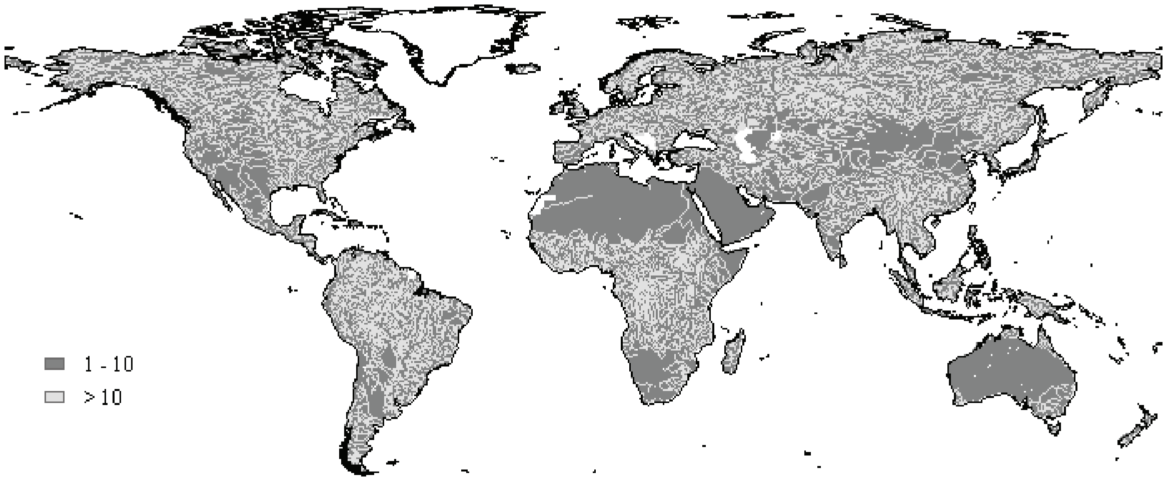

Fig. 3 Predicted values of global dilution factor (*DF*) at 0.5° × 0.5° resolution.

RESULTS AND DISCUSSION

The spatial distribution of *DF* values calculated using equation (5) is shown in Fig. 3.

Large areas with low *DF* values are visible in the western half of North America, the Pampas of Argentina, North Africa and the Middle East, parts of central Asia, Australia and southern Africa. Values of *DF* in the equatorial belt and in most of northern Europe, Canada and Siberia are generally high. Within the methodology described here, *DF* can be influenced by two main factors: (a) surface water discharge, and (b) population density and domestic water use. Low values can be due to either arid conditions or very high population density (or both). It should be noted that low values of *DF* do not necessarily represent areas of high risk in receiving environments resulting from chemical emissions. For example, in the case of some very arid regions (e.g. the Sahara desert), both runoff and population density may be very low resulting in low values of *DF*. However, the impact of emissions on surface waters in these systems may not be significant because of negligible wastewater flow.

There are a number of ways in which the cell-based estimates of *DF* can be used. Often, environmental management (and associated risk assessments) is conducted on a national basis. For screening-level PEC assessments, a single statistic of *DF* (e.g. the mean or a percentile value) for an individual country may be required. However, the use of mean values on their own may be misleading, particularly for large countries with a high degree of spatial variability in population density and climate. The use of mapped values such as those presented here, which could include the influence of flow seasonality, provide a better picture of the geographical distribution of *DF*. This information would be required in probabilistic approaches to risk assessment (e.g. Feijtel *et al.*, 1999).

The following factors are not explicitly considered in the methodology presented here but are likely to be important in determining actual PECs locally: wastewater treatment provision (and consequent chemical removal); in-sewer and in-stream losses (e.g. adsorption to sediment and volatilization); and the possibility that certain products are used more intensively on certain days. Where suitable data are available these factors might be considered in more detailed (and more realistic) risk assessments.

Further work is required to develop the proposed methodology. This includes more rigorous testing of the hydrological predictions with respect to gauged flows from around the world, including the effects of flow seasonality and the mitigating role of groundwater discharge. It is possible that the suitability of the hydrological model employed will vary from region to region. In some cases it may be necessary to apply different models to different regions of the world with the distribution of runoff globally derived from a composite of outputs from several models.

CONCLUSIONS

This paper describes a methodology which, for the first time, allows consistent, hydrologically-based environmental risk assessments for "down-the-drain" chemicals discharged to freshwaters to be performed in any country in the world. The methodology represents an intermediate level model between generic multi-media models (e.g. EC, 2003) and detailed spatially referenced catchment-scale models, such as GREAT-ER (Feijtel *et al.*, 1997). Such an intermediate-level assessment can help to identify particular regions where chemical concentrations in surface waters may be a cause for concern and, thus, provide a means of targeting more detailed local-scale risk assessments and risk management measures where necessary.

Acknowledgements We would like to thank the providers of all the data utilised in this paper, without whom this analysis would not have been possible. We also thank Dr Henry King of Unilever for helpful comments on the manuscript.

REFERENCES

Abdulla, F. A. & Lettenmaier, D. P. (1997) Application of regional parameter estimation schemes to simulate the water balance of a large continental river. *J. Hydrol.* **197**(1–4), 258–285.

Alcamo, J., Doll, P., Henrichs, T., Kaspar, F., Lehner, B., Rosch, T. & Siebert, S. (2003) Global estimates of water withdrawals and availability under current and future "business-as-usual" conditions. *Hydrol. Sci J.* **48**(3), 339–348.

Arnell, N. W. (1999) A simple water balance model for the simulation of streamflow over a large geographic domain. *J. Hydrol.* **217**(3–4), 314–335.

Edwards, M. (1989) Global Gridded Elevation and Bathymetry (ETOPO5), Digital Raster Data on a 5-minute Geographic Grid.: NOAA National Geophysical Data Center, Boulder, Colorado, USA.

European Commission (EC) (2003) Technical guidance document on Risk Assessment in Support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances, Commission regulation (EC) no. 1488/94 on Risk Assessment for Existing Substances, and Directive 98/8/EC of the European Parliament and of the Council Concerning the Placing of Biocidal Products on the Market. Part II. Office for Official Publications of the European Communities.

FAO/UNESCO (1986) Gridded FAO/UNESCO Soil Units. UNEP/GRID, FAO Soil Map of the World in Digital Form, Digital raster data on 2 minute Geographic (lat × lon) 5400 × 10800 grid. UNEP/GRID, Carouge, Switzerland.

Feijtel, T., Boeije, G., Matthies, M., Young, A., Morris, G., Gandolfi, C., Hansen, B., Fox, K., Holt, M. & Koch, V. (1997) Development of a Geography-referenced Regional Exposure Assessment Tool for European Rivers – GREAT-ER contribution to GREAT-ER #1. *Chemosphere* **34**(11), 2351–2373.

Feijtel, T. C. J., Struijs, J. & Matthijs, E. (1999) Exposure modeling of detergent surfactants - Prediction of 90th-percentile concentrations in the Netherlands. *Environ. Toxicol. Chem.* **18**(11), 2645–2652.

Fekete, B. M., Vorosmarty, C. J. & Grabs, W. (1999) Global, Composite Runoff Fields on Observed River Discharge and Simulated Water Balances. GRDC Report no. 22. Global Runoff Data Centre, Koblenz, Germany.

Food and Agriculture Organisation of the United Nations (FAO) (2000) AQUASTAT database. http://www.fao.org/ag/agl/aglw/aquastat/dbase/index2.jsp, FAO's Land and Water Development division website.

Gleick, P. H. (1996) Basic water requirements for human activities: Meeting basic needs. *Water International* **21**(2), 83–92.

Legates, D. R. & Willmott, C. J. (1990) Mean Seasonal and Spatial Variability in Gauge-Corrected, Global Precipitation. *Int. J. Climatol.* **10**(2), 111–127.

Melillo, J. M., McGuire, A. D., Kicklighter, D. W., Moore, B., Vorosmarty, C. J. & Schloss, A. L. (1993) Global Climate-Change and terrestrial net primary production. *Nature* **363**(6426), 234–240.

Nijssen, B., Lettenmaier, D. P., Liang, X., Wetzel, S. W. & Wood, E. F. (1997) Streamflow simulation for continental-scale river basins. *Water Resour. Res.* **33**(4), 711–724.

Olson, J. S. I. (1992) World Ecosystems (WE1.4). Digital Raster Data on a 10-minute Cartesian Orthonormal Geodetic 1080 × 2160 grid. n: Global Ecosystems Database, version 2.0. National Geophysical Data Center, Boulder, Colorado, USA.

Organisation for Economic Co-operation and Development (OECD) (2002) OECD Environmental Data—Compendium 2002. http://www.oecd.org/dataoecd/8/19/2958157.pdf, OECD website.

SEDAC (Socioeconomic Data and Applications Center) (2000) Gridded population of the world (v2). http://sedac.ciesin.columbia.edu/plue/gpw/index.html?main.html&2, Center for International Earth Science Information Network (CIESIN) website.

World Resources Institute (WRI) (2003) Water Resources and Freshwater Ecosystems – Freshwater Resources 2003. http://earthtrends.wri.org/datatables/index.cfm?theme=2, WRI EarthTrends Environmental Information Portal.