Chapter 12
Computational Techniques Application in Environmental Exposure Assessment

Karolina Jagiello
University of Gdansk, Poland

Tomasz Puzyn
University of Gdansk, Poland

ABSTRACT

In this chapter, the application of computational techniques in environmental exposure assessment was described. The most important groups of these techniques are Multimedia Mass-balance (MM) modelling and Quantitative Structure-Activity/Structure-Property Relationships (QSAR/QSPR) modelling. Multimedia Mass-balance models have been widely utilized for studying Long-Range Transport Potential (LRTP) and overall persistence (P_{OV}) of Persistent Organic Pollutants (POPs), regulated by many national and international acts, including the Stockholm Convention on POPs. Recently, a novel modelling methodology that links QSPR and MM has been implemented. According to this approach, the physical/chemical properties required as the input variables for multimedia modelling can be calculated directly from appropriate QSPR models. QSPR models must be previously developed based on the relationships between the chemical structure and the modelled properties (QSPR).

INTRODUCTION

The commercialisation of new products that contain growing volumes of various chemical compounds, is the result of progress in civilisation. Certain chemicals, however, may have a negative impact on the human body and natural environment. Furthermore, noxious chemical compounds may be generated as the side products of the manufacturing processes. Consequently, development of reliable methods of risk assessment, which would allow eliminating potentially dangerous chemical substances at the stage of synthesis or final product planning, seems to be increasingly essential. Such methods should ensure good pace and cost-efficiency so as to avoid additional expenses.

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The provisions contained in the REACH Regulation (EC, 2006) that requires the entities to file every new chemical substance to be commercialised on the European market in large quantities (either manufactured or imported) with the European Chemicals Agency in Helsinki, Finland, have applied to the European Union countries since recently. The registration process must be preceded by the phase of evaluation of the chemical risk. Article 13 of the REACH Regulation determines that information on the substance should be generated, if only possible, using so called "alternative methods" with regard to ethically doubtful and expensive tests on animals. Computer assisted methods, specifically those using the quantitative modelling of relationships between the chemical structure and activity (Quantitative Structure-Activity Relationships, QSAR) and physical properties (Quantitative Structure-Property Relationships, QSPR) may be listed from among "alternative methods".

Special attention is given to the chemical substances which are defined by the acronym PBT (Persistent, Bioaccumulative and Toxic) and classified as: persistent (P), bioaccumulative (B), and toxic (T) either in the European REACH Regulation or in the legislation concerning chemical safety and applicable to Canada (CEPA, 1999), United States of America (USEPA, 1999), or Japan (METI, 1973). It should be mentioned here that the criteria of eligibility of a substance for PBT, Table 1, originate from previous research into the group of Persistent Organic Pollutants (POPs) (Gobas, 2009; van Wijk, 2009). The awareness of the risk connected with the presence of POPs in the natural environment at the turn of the 1960's and 1970's allowed launching many initiatives of multinational nature, with the aim to decrease the production and usage of such substances in order to reduce the emissions of chemical pollutants. In this context, POPs may be considered as "model pollutants" the tests of which have allowed developing many theories of transport and deposits in natural environment as well as toxicity and ecotoxicity of pollutants, such theories being largely applied these days. Recently, more and more attention is given to brominated and bromochlorinated POPs (Br-POPs and Br/Cl-POPs) given their increasing emissions to the environment and high levels of Br-POPs and Br/Cl-POPs observed in environmental matrices (Batterman, 2007; Du, 2010; Hutson, 2009), as well as their confirmed toxicity (Birnbaum, 2003).

The present chapter describes the existing scientific knowledge in two areas of concern, that is:

1. Fundamental elements of QSAR/QSPR methodologies, and
2. Development of the methodology of predicting transport of chemical substances in the environment on the basis of combination of Multimedia Mass Balance Models (MM) with QSPR models (QSPR-MM hybrid models).

BASIC IDEA AND INCREASING IMPORTANCE OF QSPR/QSAR METHODS

QSAR/QSPR models rely on a shared assumption that the variance of modelled quantity **y** (either physical/chemical property or biological activity, respectively) in a group of chemical compounds featuring similar structures is determined by the variance connected with differences in chemical structure of such compounds, whereas the mutability of chemical structure is expressed numerically by means of structural descriptors **X**. Hence, if we have experimentally measured values of a physical/chemical quantity or of activity **y** for a suitably number of compounds as well as the values of structural descriptors **X** for all the compounds, we will be able to build a suitable model in the format shown in Equation (1).

$$y = f(X). \tag{1}$$