

Livello Quarto: Distribuzioni in stato non stazionario

Per composti che subiscono modifiche ambientali di idrolisi, ossidazione ecc. e la cui emissione nell'ambiente è cessata ad un certo tempo.

Valutare la loro persistenza e quanto tempo necessita perché si instaurino concentrazioni di un certo valore (limiti e/ o standard di qualità).

$$fugacità = f(t)$$

Inserire la componente *tempo* per verificare i cambiamenti della fugacità in relazione alla scomparsa dell'inquinante conseguente alle *reazioni ambientali* ed ai *trasferimenti*.

Il IV Livello descrive le variazioni delle concentrazioni e delle fugacità

- ❑ dal momento 0 (si presume l'assenza dell'inquinante)
- ❑ fino al momento in cui si sono raggiunte condizioni di equilibrio temporanee tra entrate ed uscite (Livello III) e, successivamente
- ❑ diminuzione della sostanza dopo che è stata interrotta l'emissione.

Il IV Livello potrebbe essere adottato per conoscere le dinamiche di recupero ambientale dopo che si è interrotta una certa emissione inquinante.

Livello IV

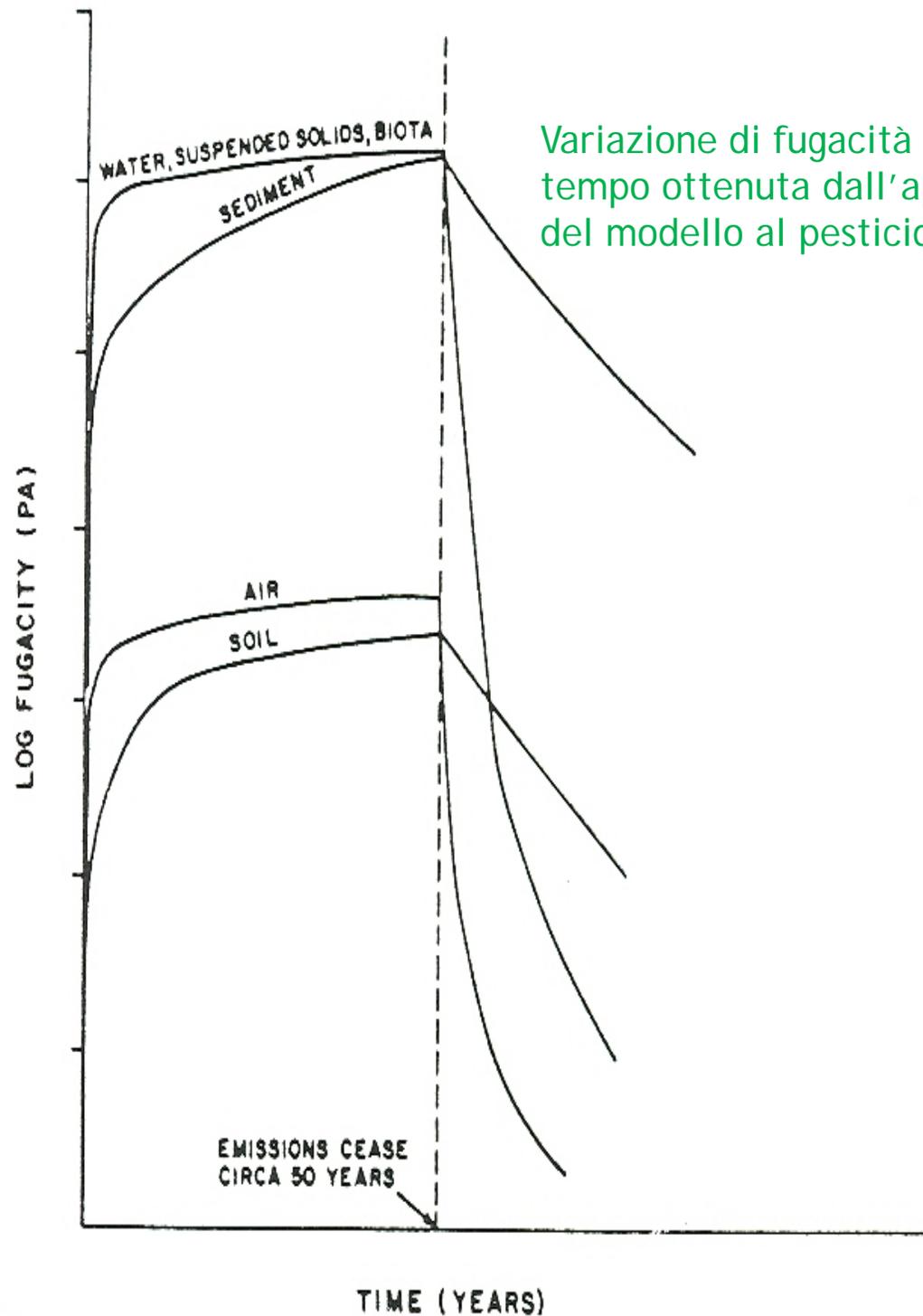
= descrizione del comportamento di una sostanza in un sistema non in equilibrio e in stato non stazionario.

Sistema di equazioni differenziali che descrivono la variazione di concentrazione nei vari comparti rispetto al tempo.

Per ciascun comparto si può scrivere:

$$V_i \frac{dC_i}{dt} = V_i Z_i D \frac{df_i}{dt} = E_i - f_i V_i Z_i k_i - \sum_j D_{ij} f_i + \sum_j D_{ji} f_j$$

Questa equazione permette di considerare immissioni che variano nel tempo e di determinare sia il tempo necessario per raggiungere lo stato stazionario sia il tempo di decadimento dopo la riduzione delle immissioni. Questi dati sono utili per la previsione della contaminazione a lungo termine di prodotti nuovi o già esistenti



Variazione di fugacità rispetto al tempo ottenuta dall'applicazione del modello al pesticida Mirex.

Esempi

Application of a level IV fugacity model to simulate the long-term fate of hexachlorocyclohexane isomers in the lower reach of Yellow River basin, China

Chemosphere 74 (2009) 370–376

The Yellow River is the second largest river in China, with a total length of 5464 km. The lower reach of the Yellow River extends 786 km from Huayuankou through the flat alluvial plains of Henan and Shandong provinces to the river mouth, with a basin area of $2.261 \times 10^4 \text{ km}^2$ (Liu et al., 1997; He, 2000; Wang et al., 2007), accounting for 3% of the whole area of the Yellow River basin. The lower basin is a humid area, with annual average temperature of 12–14 °C, and annual average precipitation of 670 mm (Wang et al., 2007). The light and heat resources are very abundant in the basin, and the natural conditions make it an agriculturally fertile area for many kinds of crops.

A level IV fugacity model based on a non-steady-state assumption was applied to simulate the temporal trends of concentrations and inter-compartmental transfer fluxes of HCHs from 1952 to 2010. Air (pure air and particulates), water (pure water and suspended solids), soil (air, water and solids), and sediment (water and solids) were the four bulk compartments included in the fugacity model. The processes taken into consideration in the model for HCHs included agricultural application, advection air/water flow in/out of area, exchange between inter-compartment, and degradation in the four bulk compartments.

the non-steady-state mass bal-

ance of HCH isomers in the four compartments was described with the following system of linear differential equations:

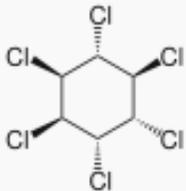
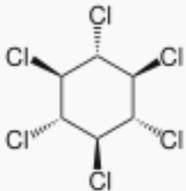
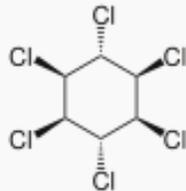
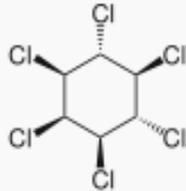
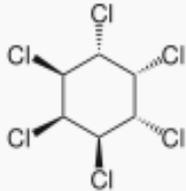
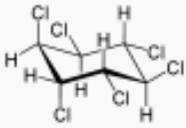
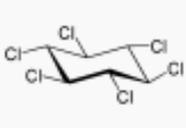
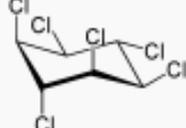
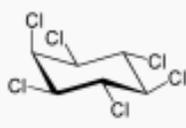
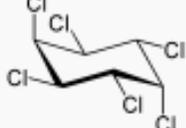
$$V_A Z_A \frac{df_A}{dt} = E_A + G_A C_A + D_{W-A} f_W + D_{S-A} f_S - (D_{A-W} + D_{A-S} + D_{A(A)} + D_{R(A)}) f_A \quad (1)$$

$$V_W Z_W \frac{df_W}{dt} = G_W C_W + D_{A-W} f_A + D_{S-W} f_S + D_{Sed-W} f_{Sed} - (D_{W-A} + D_{W-Sed} + D_{A(W)} + D_{R(W)}) f_W \quad (2)$$

$$V_S Z_S \frac{df_S}{dt} = E_S + D_{A-S} f_A - (D_{S-A} + D_{S-W} + D_{R(S)}) f_S \quad (3)$$

$$V_{Sed} Z_{Sed} \frac{df_{Sed}}{dt} = D_{W-Sed} f_W - (D_{Sed-W} + D_{R(Sed)}) f_{Sed} \quad (4)$$

Esaclorocicloesani

Nome	α -esaclorocicloesano	β -esaclorocicloesano	γ -esaclorocicloesano	δ -esaclorocicloesano	ε -esaclorocicloesano
Formula di struttura					
Struttura spaziale (per l'isomero α sono mostrati anche gli atomi d'idrogeno)					
Numero CAS			Miscela isomerica 608-73-1		
Numero CAS	319-84-6	319-85-7	58-89-9	319-86-8	6108-10-7
PubChem			727 		
Formula bruta			$C_6H_6Cl_6$		
Massa molecolare			290,83 g·mol ⁻¹		
Stato della materia			solido		
Descrizione breve	Sostanza solida tra il giallino e il trasparente dall'odore di muffa				
Punto di fusione	159-160 °C ^[3]	309 °C ^[4]	113 °C ^[5]	139 °C ^[6]	
Punto di ebollizione	288 °C ^[3]		323 °C (Degradazione) ^[5]		
Densità		1,89 g/cm ³ ^[4]	1,85 g/cm ³ ^[5]	1,55 g/cm ³ ^[6]	
Solubilità	Minimamente solubile in acqua (0,2–8 mg/l) ^{[3][4][5][6]}				
Rischio chimico ^{[3][4][5][6]}					
Frase R	Template:Frase-R		Template:Frase-R	Template:Frase-R	
Frase S	Template:Frase-S		Template:Frase-S	Template:Frase-S	

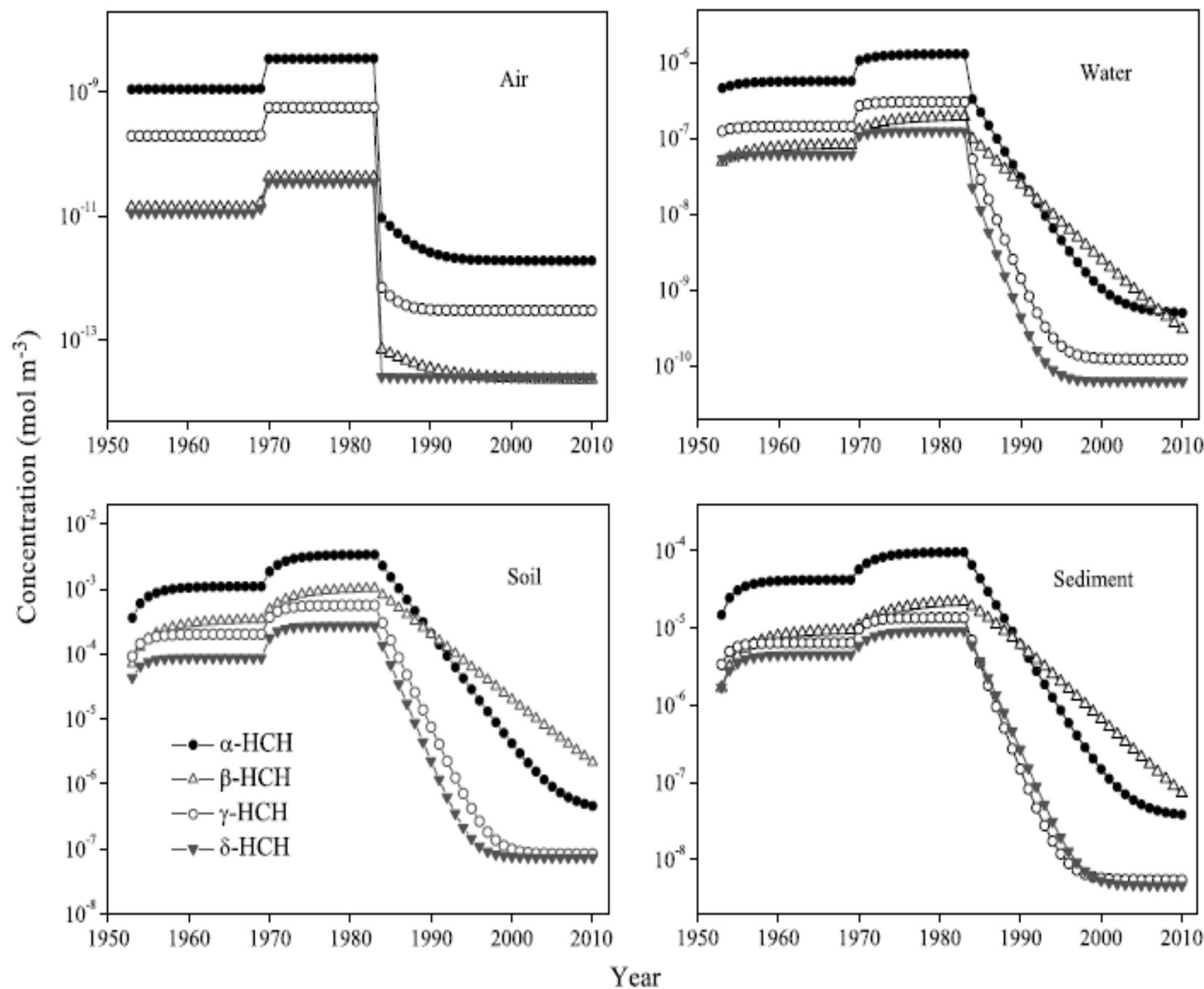


Fig. 1. Temporal trends of the concentration of HCH isomers in various compartments from 1952 to 2010.

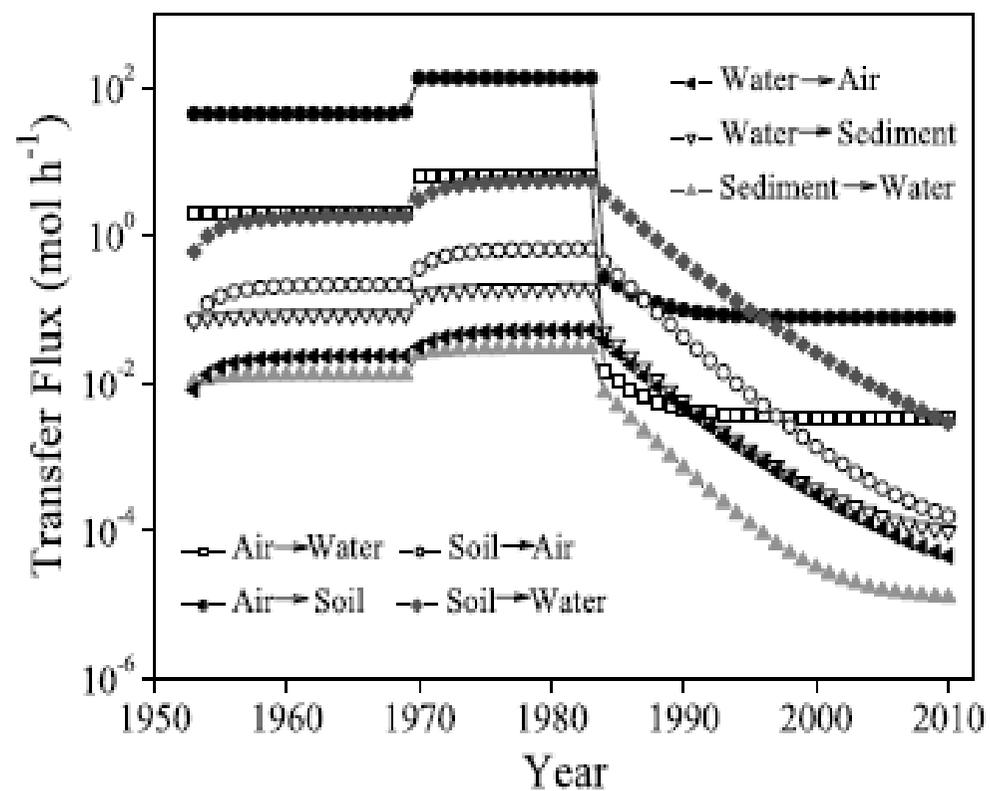
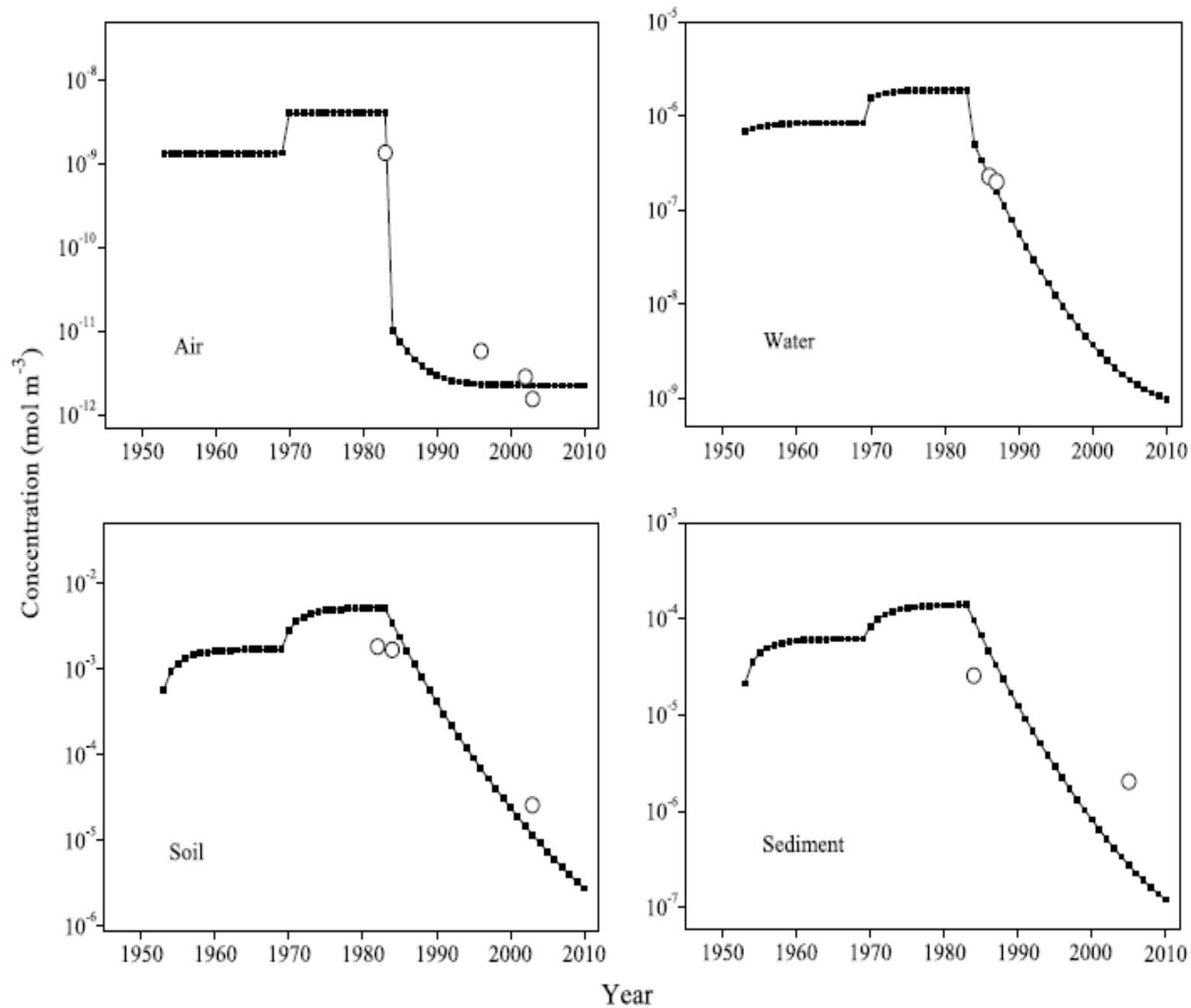


Fig. 2. Transfer fluxes of HCHs between the adjacent compartments during 1952–2010.



. Comparison between the calculated (curve) and observed (dot) concentrations of HCHs in various compartments in different periods.



Available online at www.sciencedirect.com



Computers and Mathematics with Applications 56 (2008) 657–669

An International Journal
**computers &
mathematics**
with applications

www.elsevier.com/locate/camwa

Modelling the pesticide concentration in a rice field by a level IV fugacity model coupled with a dispersion-advection equation

Wilson A. Contreras^{a,b,*}, Damián Ginestar^b, Lourival C. Paraíba^c, Rafael Bru^b

^a *Mathematics Department, Faculty of Basic Sciences, University of Pamplona, Km 1 way Bucaramanga, Colombia*

^b *Instituto de Matemática Multidisciplinar, Universidad Politécnica de Valencia, 46022, Valencia, Spain*

^c *EMBRAPA Meio Ambient, Rodovia Campinas Mogi-Mirim, SP 340 km 127.5. CxP: 69. CEP 13820-000.Jaguariúna (São Paulo), Brazil*



Available online at www.sciencedirect.com



Chemosphere 70 (2008) 607–615

CHEMOSPHERE

www.elsevier.com/locate/chemosphere

Development of a black carbon-inclusive multi-media model: Application for PAHs in Stockholm

Konstantinos Prevedouros^a, Anna Palm-Cousins^b, Örjan Gustafsson^a, Ian T. Cousins^{a,*}

^a *Department of Applied Environmental Science (ITM), Stockholm University, SE-10691 Stockholm, Sweden*

^b *IVL, Swedish Environmental Research Institute Ltd., Box 21060, 100 31 Stockholm, Sweden*

Received 26 February 2007; received in revised form 29 June 2007; accepted 3 July 2007

Available online 21 August 2007