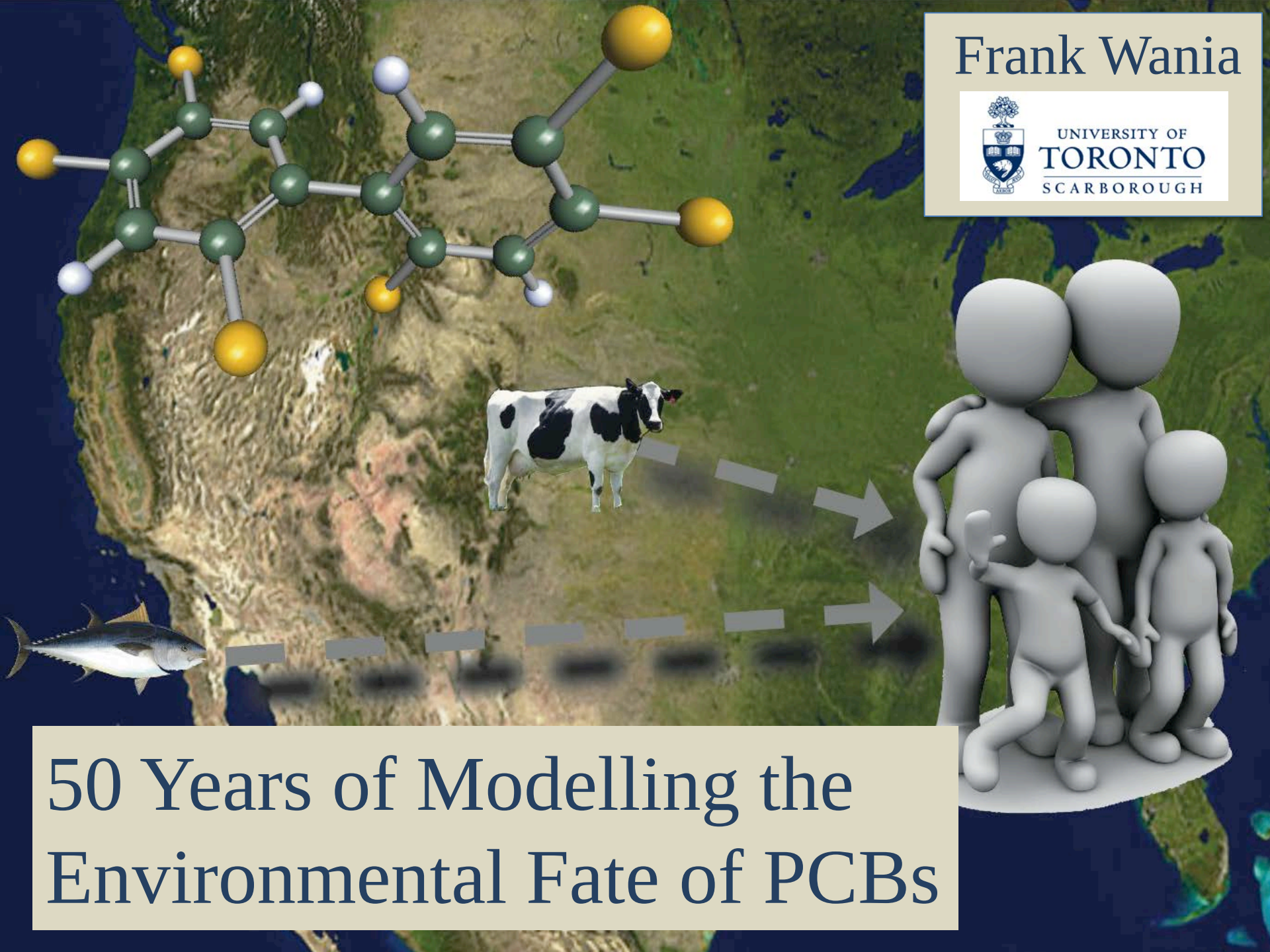
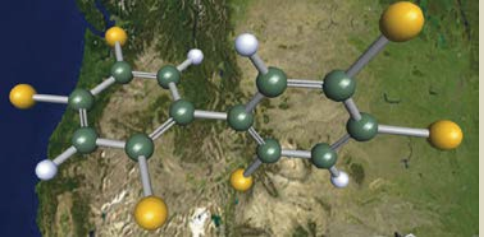


Frank Wania

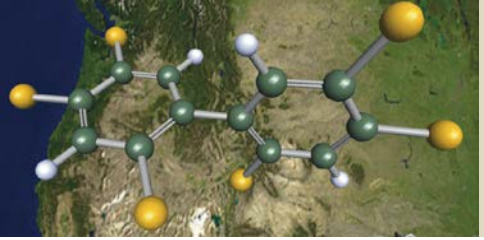
UNIVERSITY OF TORONTO SCARBOROUGH

50 Years of Modelling the Environmental Fate of PCBs



Modelling the Environmental Fate of PCBs

PCBs have been the favorites of the organic contaminant modelling community for a long time



Modelling Fate in the **Physical Environment**

MODELING THE LONG-TERM BEHAVIOR OF AN ORGANIC CONTAMINANT IN A LARGE LAKE: APPLICATION TO PCBs IN LAKE ONTARIO

Donald Mackay
Institute for Environmental Studies
University of Toronto
Toronto, Ontario M5S 1A4

Model of the Long-Term Exchange of PCBs between Soil and the Atmosphere in the Southern U.K.

TOM HARNER AND DON MACKAY*
Department of Chemical Engineering & Applied Chemistry, University of Toronto, Toronto, Ontario, M5S 1A4 Canada

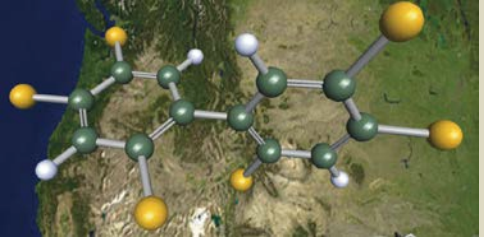
KEVIN C. JONES
Institute of Environmental and Biological Sciences, Lancaster University, Lancaster, LA1 4YQ, U.K.

The Origin and Significance of Short-Term Variability of Semivolatile Contaminants in Air

MATTHEW MACLEOD,*,† MARTIN SCHERINGER,† HEIKE PODEY,† KEVIN C. JONES,‡ AND KONRAD HUNGERBÜHLER†
Institute for Chemical and Bioengineering, ETH Zurich, CH-8093 Zurich Switzerland, and Centre for Chemicals

MODELING THE FATE OF POLYCHLORINATED BIPHENYLS IN THE INNER OSLOFJORD, NORWAY

KNUT BREIVIK,*† BIRGER BJERKENG,‡ FRANK WANIA,§ AUD HELLAND,‡ and JAN MAGNUSSON‡



Global Fate and Transport Modelling

Report Frank Wania and Yushan Su

Quantifying the Global Fractionation of Polychlorinated Biphenyls

Estimating the contribution of degradation in air and deposition to the deep sea to the global loss of PCBs

Frank Wania*, Gillian L. Daly

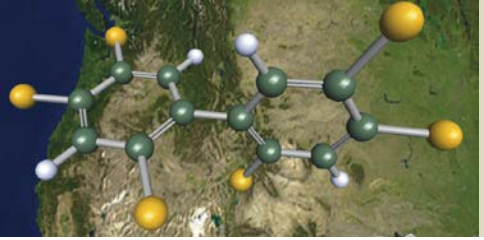
Department of Chemistry and Division of Physical Sciences, University of Toronto at Scarborough, 1265 Military Trail, Toronto, Ont., Canada M1C 1A4

Assessing the Influence of Climate Variability on Atmospheric Concentrations of Polychlorinated Biphenyls Using a Global-Scale Mass Balance Model (BETR-Global)

MATTHEW MACLEOD,*,†,‡
WILLIAM J. RILEY,§ AND
THOMAS E. MCKONE†,||

GEM/POPs: a global 3-D dynamic model for semi-volatile persistent organic pollutants – Part 2: Global transports and budgets of PCBs

P. Huang[1], S. L. Gong[1,2], T. L. Zhao[2], L. Neary[3], and L. A. Barrie[4]



Bioaccumulation Modelling

A pharmacokinetic model for the disposition of polychlorinated biphenyls (PCBs) in channel catfish

Mahesh G. Kulkarni and Adel H. Karara

Division of Pharmaceutics and Medicinal Chemistry, School of Pharmacy, Northeast Louisiana University, Monroe, LA, U.S.A.

Environ. Sci. Technol. **1991**, *25*, 760–770

Application of a Food Chain Model to Polychlorinated Biphenyl Contamination of the Lobster and Winter Flounder Food Chains in New Bedford Harbor

John P. Connolly

HydroQual, Inc., 1 Lethbridge Plaza, Mahwah, New Jersey 07430 and Environmental Engineering and Science Program, Manhattan College, Riverdale, New York 10471

Modelling Bioaccumulation of Organic Pollutants in Fish with an Application to PCBs in Lake Ontario Salmonids

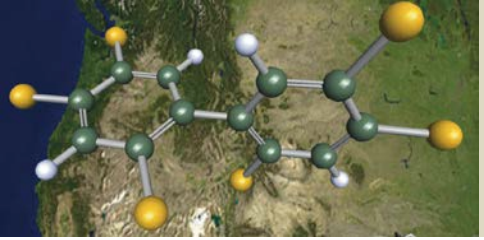
M. Craig Barber, Luis A. Suárez, and Ray R. Lassiter

Environmental Research Laboratory, U.S. Environmental Protection Agency, Athens, GA 30613, USA

Bioenergetics and PCB, DDE, and Mercury Dynamics in Lake Ontario Lake Trout (*Salvelinus namaycush*): A Model based on Surveillance Data

U. Borgmann and D. M. Whittle

Department of Fisheries and Oceans, Great Lakes Laboratory for Fisheries and Aquatic Sciences, Burlington, Ont. L7R 4A6, Canada



Human Exposure Modelling

Towards an understanding of the link between environmental emissions and human body burdens of PCBs using CoZMoMAN

Knut Breivik [a,b,*], Gertje Czub [c], Michael S. McLachlan [c], Frank Wania [d]

A Multi-Individual Pharmacokinetic Model Framework for Interpreting Time Trends of Persistent Chemicals in Human Populations: Application to a Postban Situation

Roland Ritter, Martin Scheringer, Matthew MacLeod, Urs Schenker, and Konrad Hungerbühler

Safety and Environmental Technology Group, ETH Zurich, Zurich, Switzerland

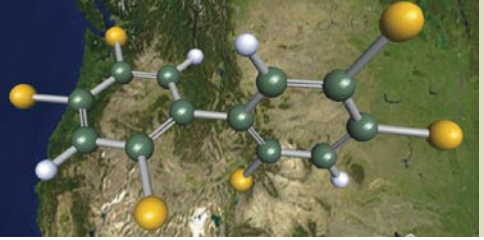
Persistent Organic Pollutants in Norwegian Men from 1979 to 2007: Intraindividual Changes, Age–Period–Cohort Effects, and Model Predictions

Therese Haugdahl Nøst,[1,2,3] Knut Breivik,[4,5] Ole-Martin Fuskevåg,[3] Evert Nieboer,[1,6] Jon Øyvind Odland,[1] and Torkjel Manning Sandanger[1,2]

[1]Department of Community Medicine, University of Tromsø, Tromsø, Norway; [2]NILU-Norwegian Institute for Air Research, Fram Centre, Tromsø, Norway; [3]University Hospital of North Norway, Tromsø, Norway; [4]NILU-Norwegian Institute for Air Research, Kjeller, ent of Biochemistry and Biomedical Sciences, McMaster

Deterministic modeling of the exposure of individual participants in the National Health and Nutrition Examination Survey (NHANES) to polychlorinated biphenyls†

Stephen A. Wood,[ab] James M. Armitage,[a] Matthew J. Binnington[a] and Frank Wania*[ab]



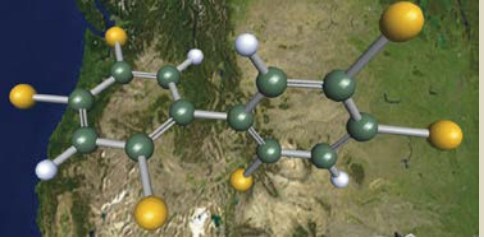
Why are PCBs the organic contaminant modellers' favorite?

Reason #1

- PCBs are a mixture of contaminants that covers an "interesting" range of
  - hydrophobicity (truly dissolved vs. sorbed to solids),
  - volatility (gas phase vs. particle bound) and
  - degradability (degradable vs. persistent)

Reason #2

- We have availability of high quality
  - partitioning and degradation properties
  - emissions



Availability of Property Data

Environ. Sci. Technol. **1988**, *22*, 382–387

Octanol–Water Partition Coefficients of Polychlorinated Biphenyl Congeners

Darryl W. Hawker* and Des W. Connell

School of Australian Environmental Studies, Griffith University, Nathan, Queensland, Australia 4111

- Congener specific
- Temperature dependent
- Consistent between congeners
- Consistent between properties

CLE/GAS
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Downsview,

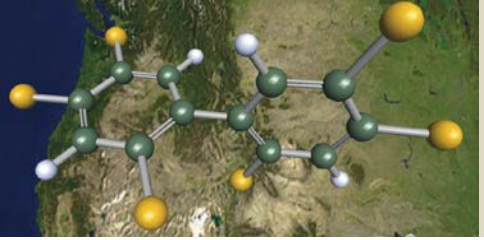
Quantitative Structure–Property Relationships for Aqueous Solubilities and Henry's Law Constants of Polychlorinated Biphenyls

Frank M. Dunnivant and Alan W. Elzerman*

Environmental Systems Engineering, Clemson University, Clemson, South Carolina 26934-0919

Peter C. Jurs and Mohamed N. Hasan

Department of Chemistry, 152 Davey Laboratory, The Pennsylvania State University, University Park, Pennsylvania 16802



Availability of Emission Data

Towards a global historical emission inventory for selected PCB congeners — a mass balance approach
1. Global production and consumption

Knut Breivik[a,*], Andy Sweetman[b], Jozef M. Pacyna[a], Kevin C. Jones[b]

Towards a

- Congener specific
- Global in Scale
- Historical in Scope

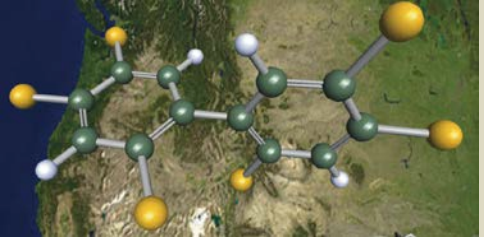
for selected PCB
ach

Knut

vin C. Jones[b]

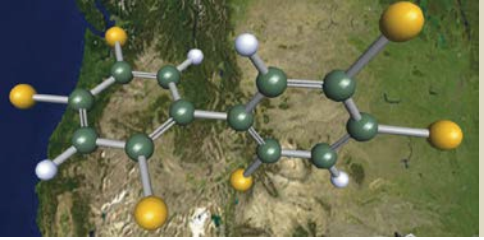
Towards a global historical emission inventory for selected PCB congeners — A mass balance approach
3. An update

Knut Breivik [a,b,*], Andy Sweetman [c], Jozef M. Pacyna [a,d], Kevin C. Jones [c]



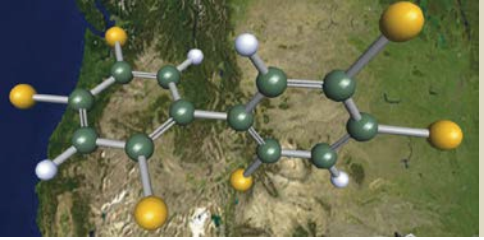
Can models provide insight?

- Given the availability of good property and emission data, what is feasible in organic contaminant modelling?
- Examples taken from human exposure modelling



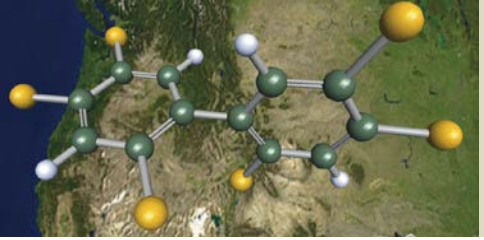
Can models provide insight?

- Why do PCB levels generally increase with age?
- When might we expect the peak in health effects caused by PCB exposure to have occurred?
- Would we expect slim or obese people to have higher PCB levels?
- When repeatedly sampling a population for human biomonitoring, do temporal changes in dietary habits and body lipids confound time trends?
- Can we reconstruct past PCB exposure in individual humans?



Can models provide insight?

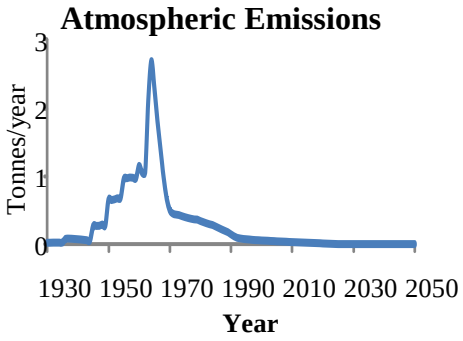
- Why do PCB levels generally increase with age in a population cross section?

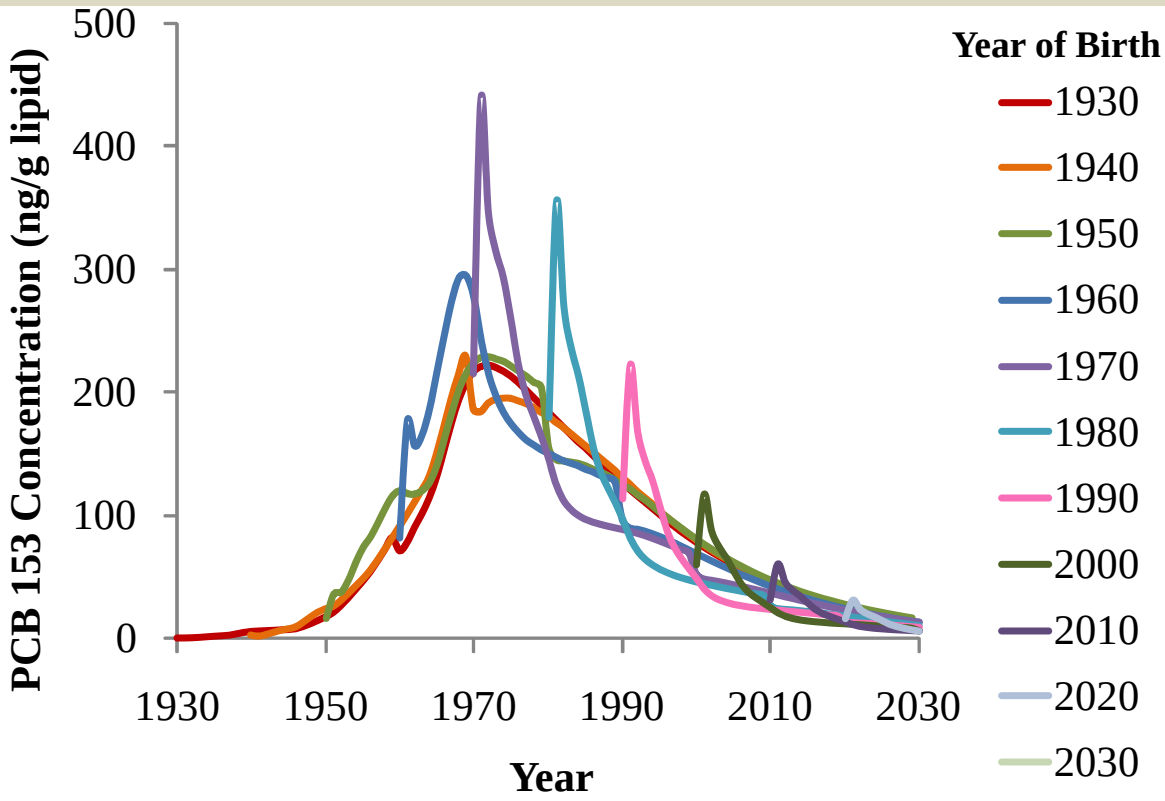


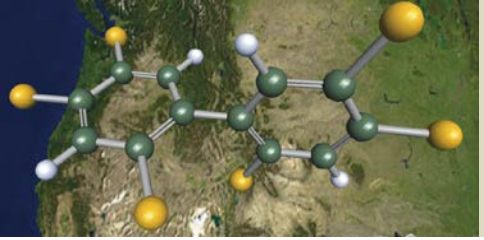
Why do PCB levels generally increase with age in a population cross section?

Example:

- PCB-153
- Sweden
- Females







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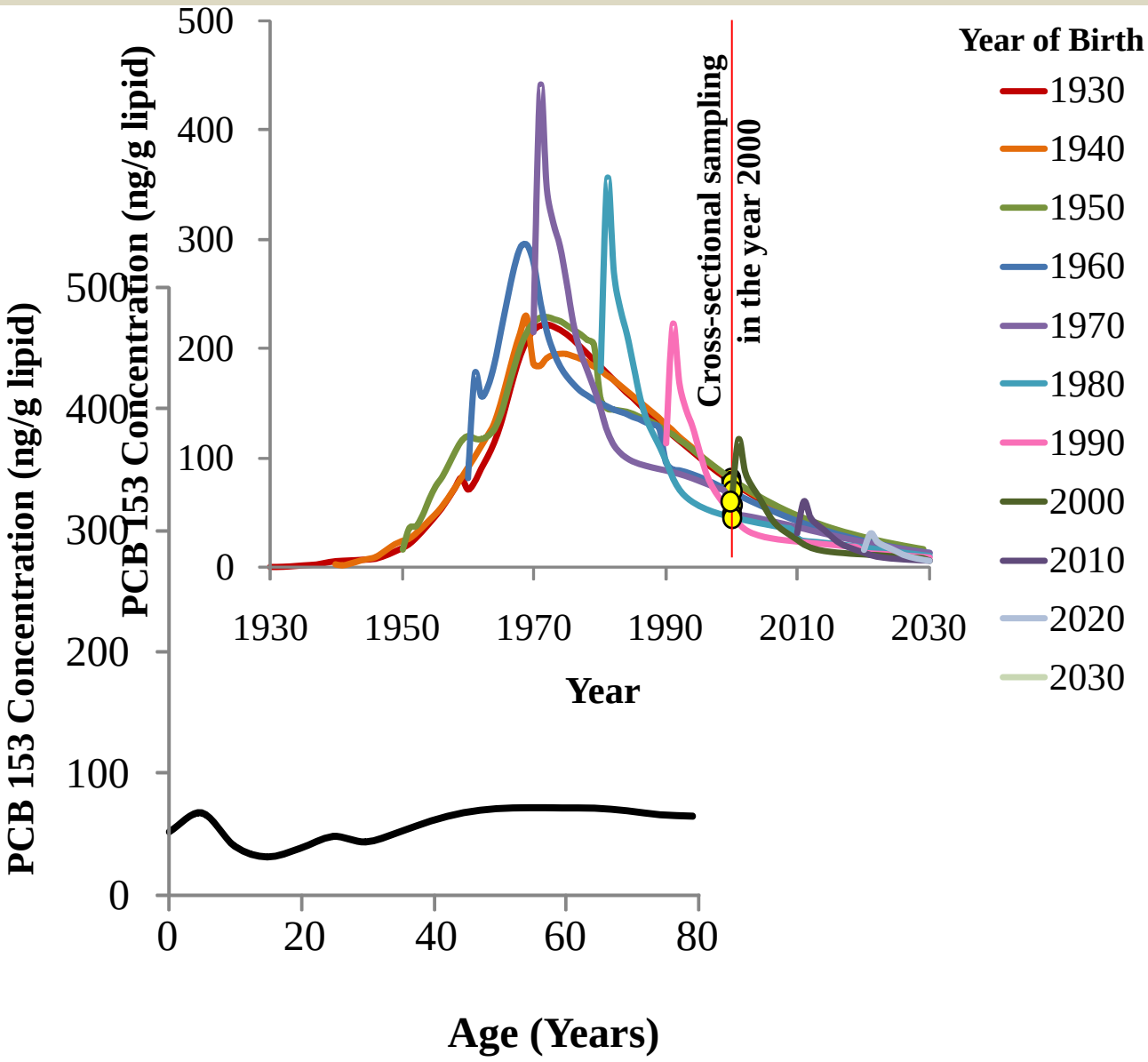

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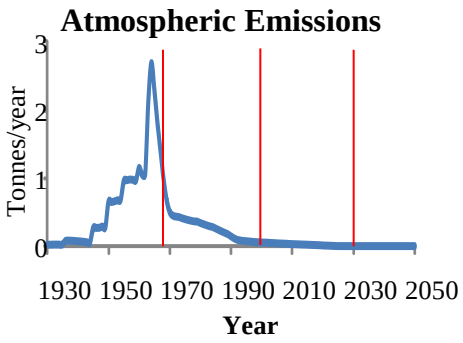
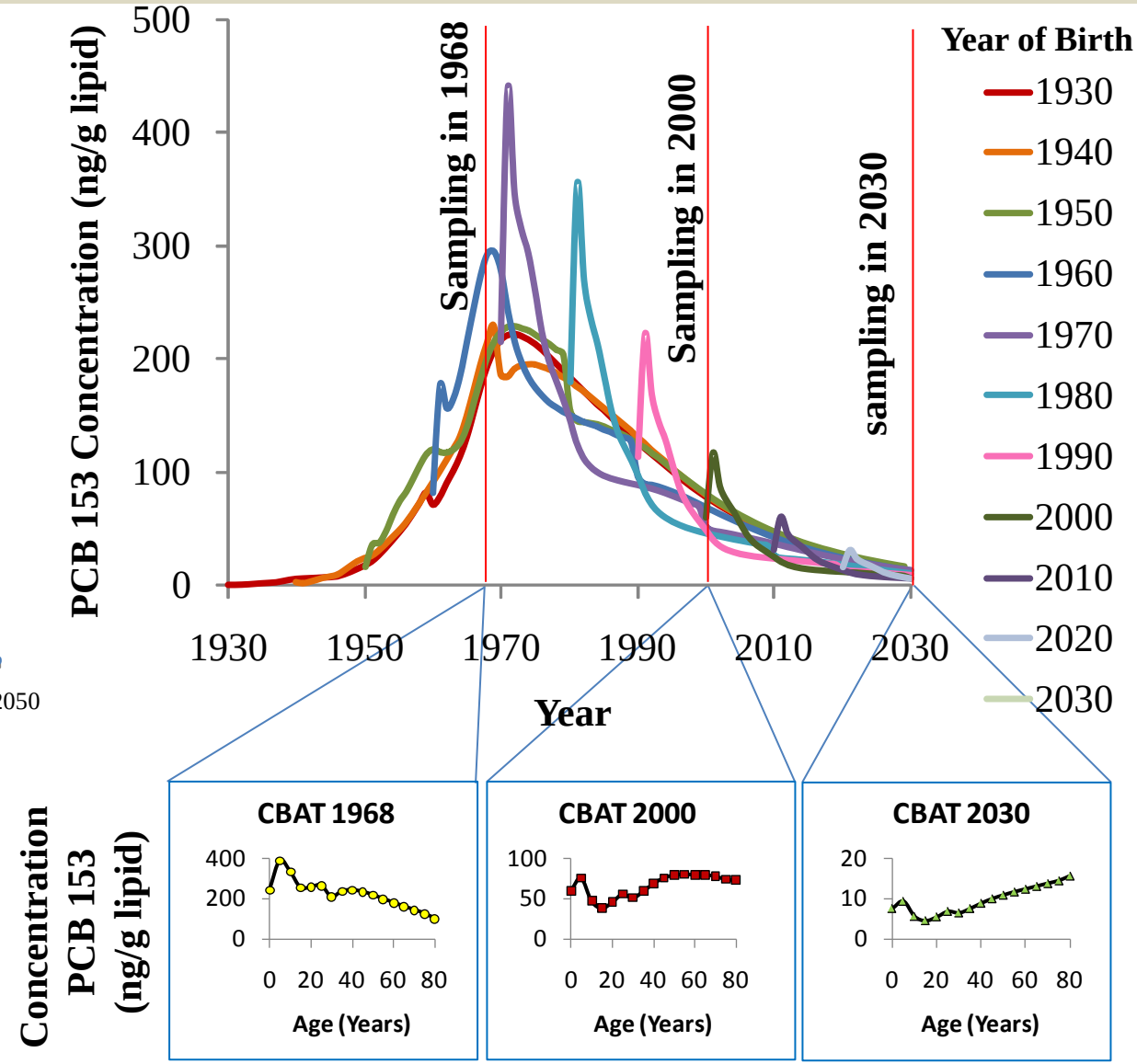
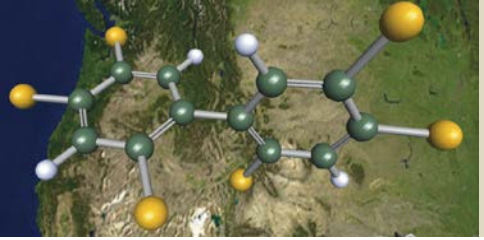


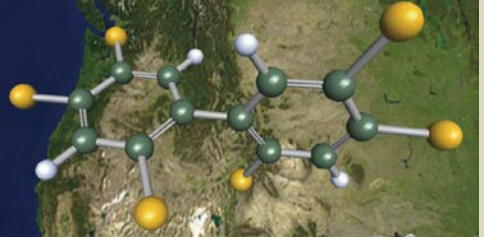




Can models provide insight?

- Why do PCB levels generally increase with age in a population cross section?
  - They do so only after emissions and therefore environmental contamination have peaked.
  - Then, older people have higher levels because their bodies retain a “memory” of higher exposure in the past?
  - During the early period of increasing contamination, children can be expected to have had higher PCB levels than adults.

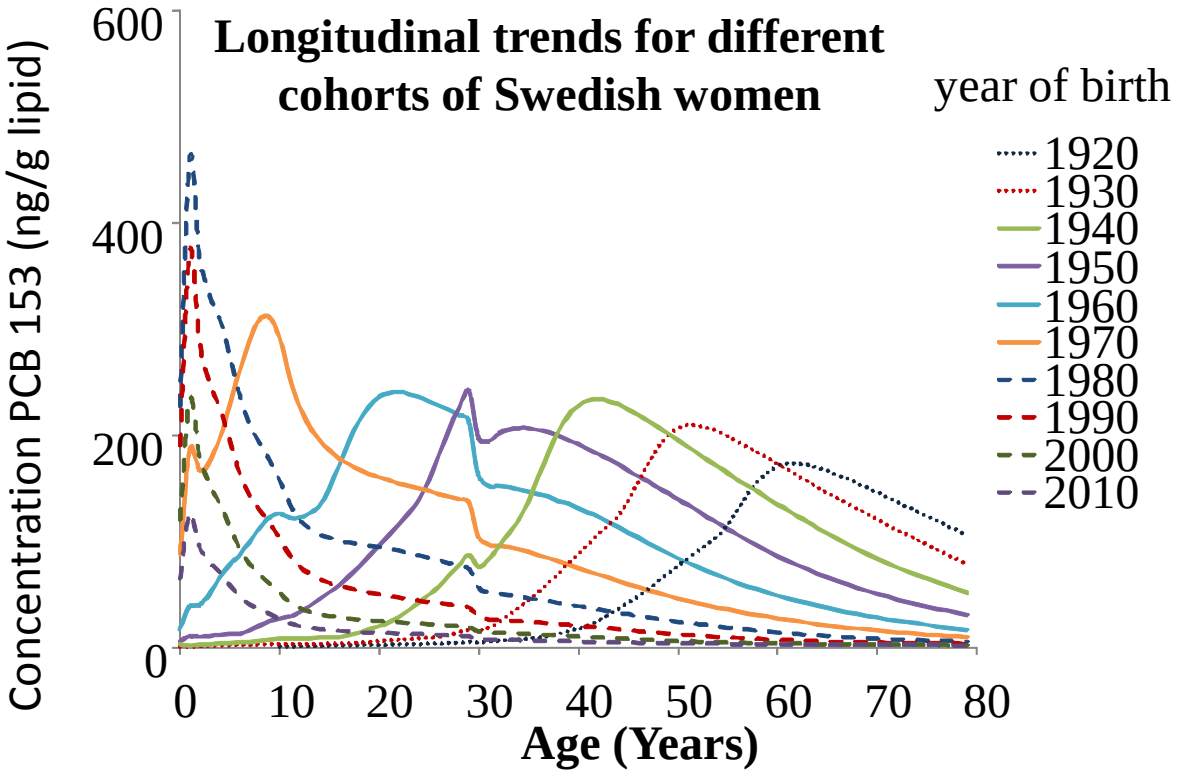
Quinn et al. *Environ. Health Persp.* **2012**, *120*, 554-559

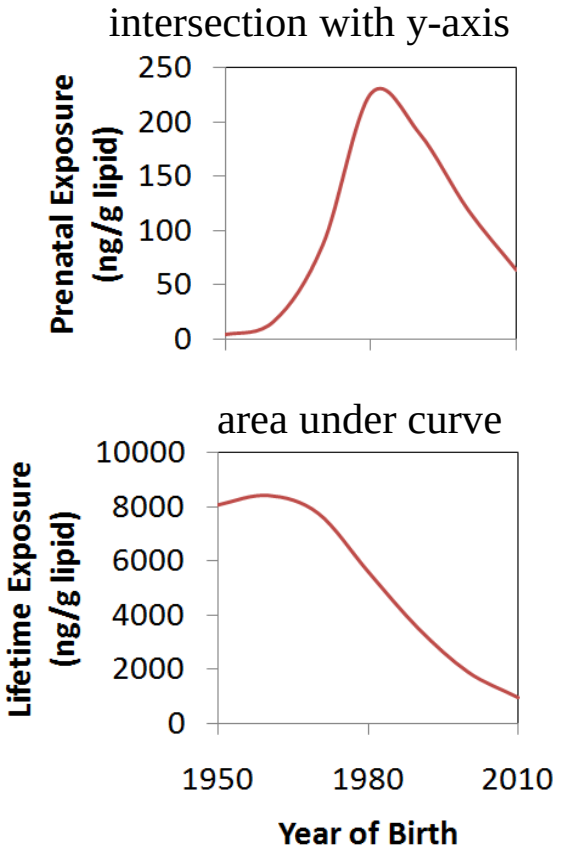


Can models provide insight?

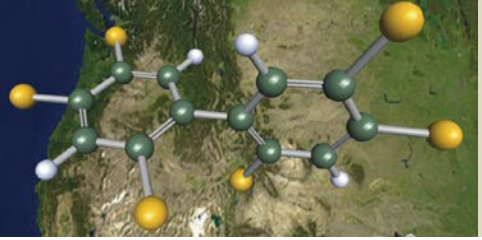
- When might we expect the peak in health effects caused by PCB exposure to have occurred?

When might we expect the peak in health effects to have occurred?



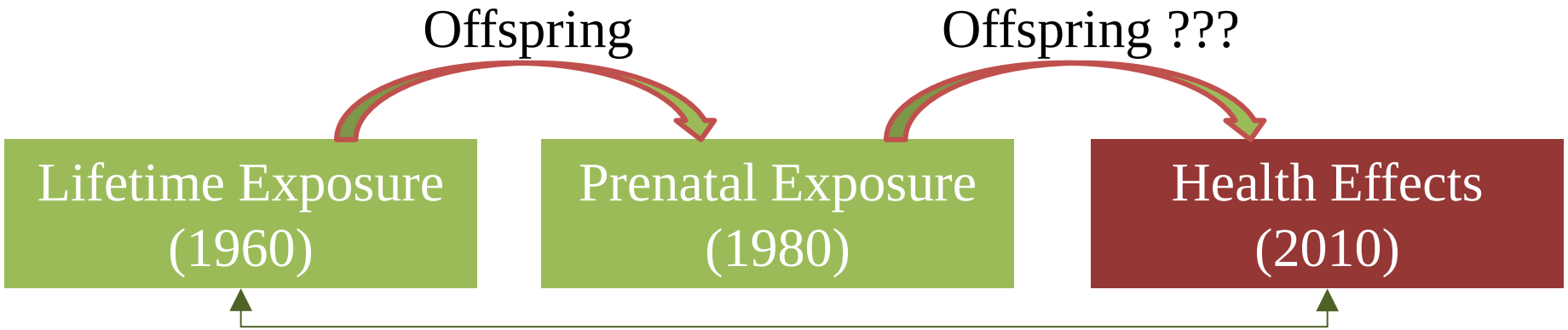


Lifetime PCB exposure was highest for those born in the 1950 and 60s.
Perinatal PCB exposure was highest for those born in 1980s and 90s.



When might we expect the peak in health effects to have occurred?

Peak in perinatal PCB exposure is delayed relative to the peak in PCB emissions

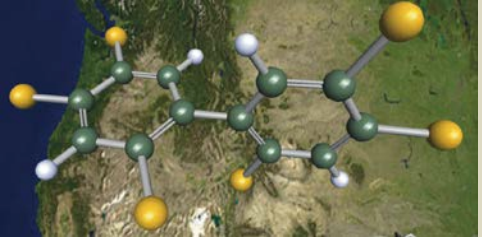


50 years (40 years since ban)

One of the health effects of perinatal exposure to PCBs is impaired ability to reproduce later in life.

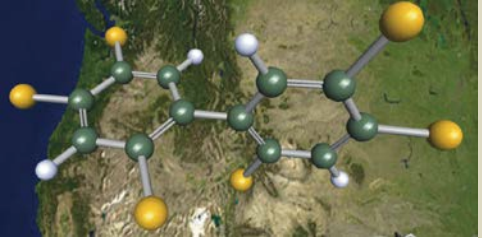
Peak in (some) health effects of PCBs exposure may occur only now!

Quinn et al. *Environ. Health Persp.* **2011**, *119*, 641-646



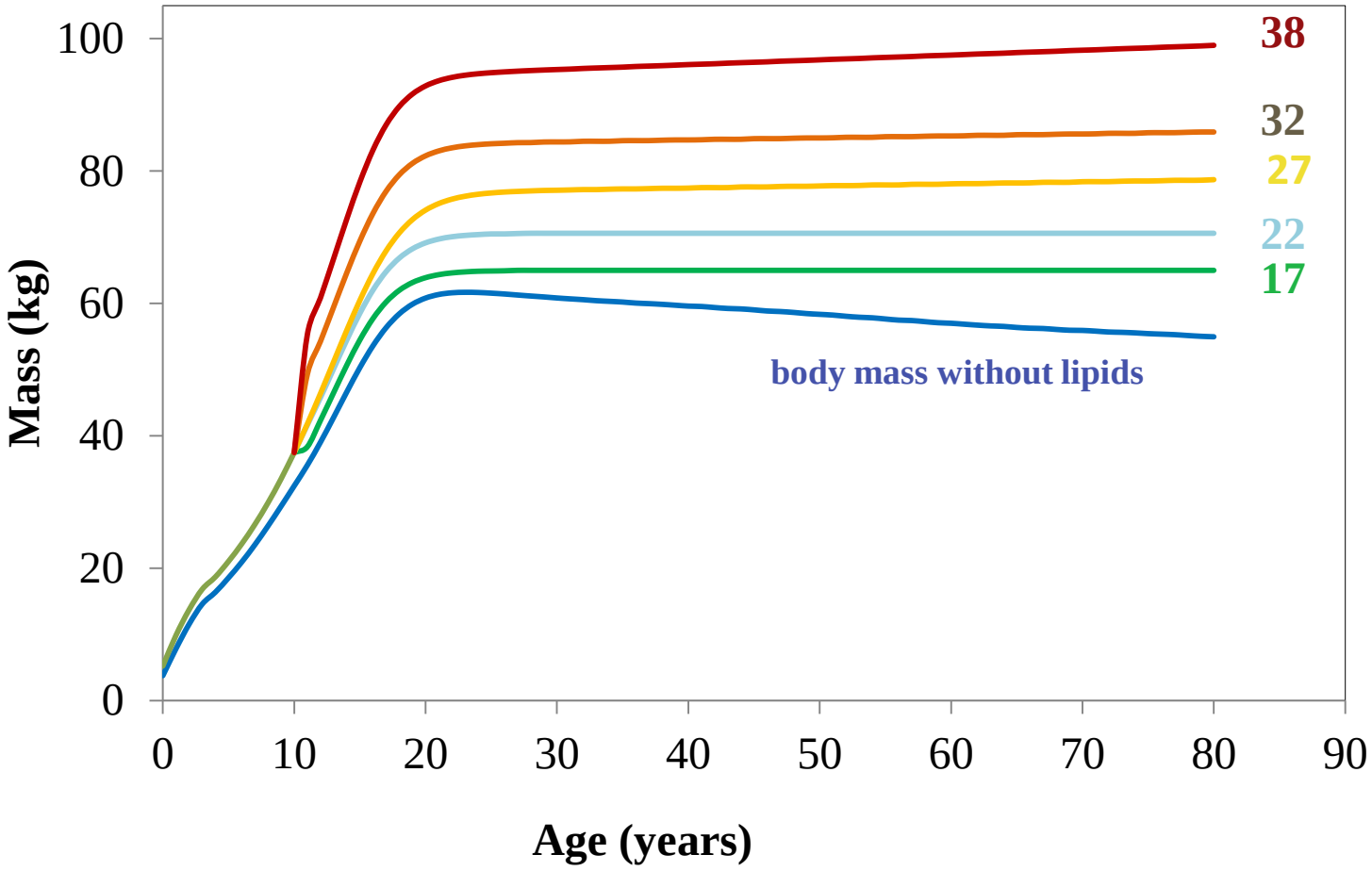
Can models provide insight?

- Would we expect slim or obese people to have higher PCB levels?



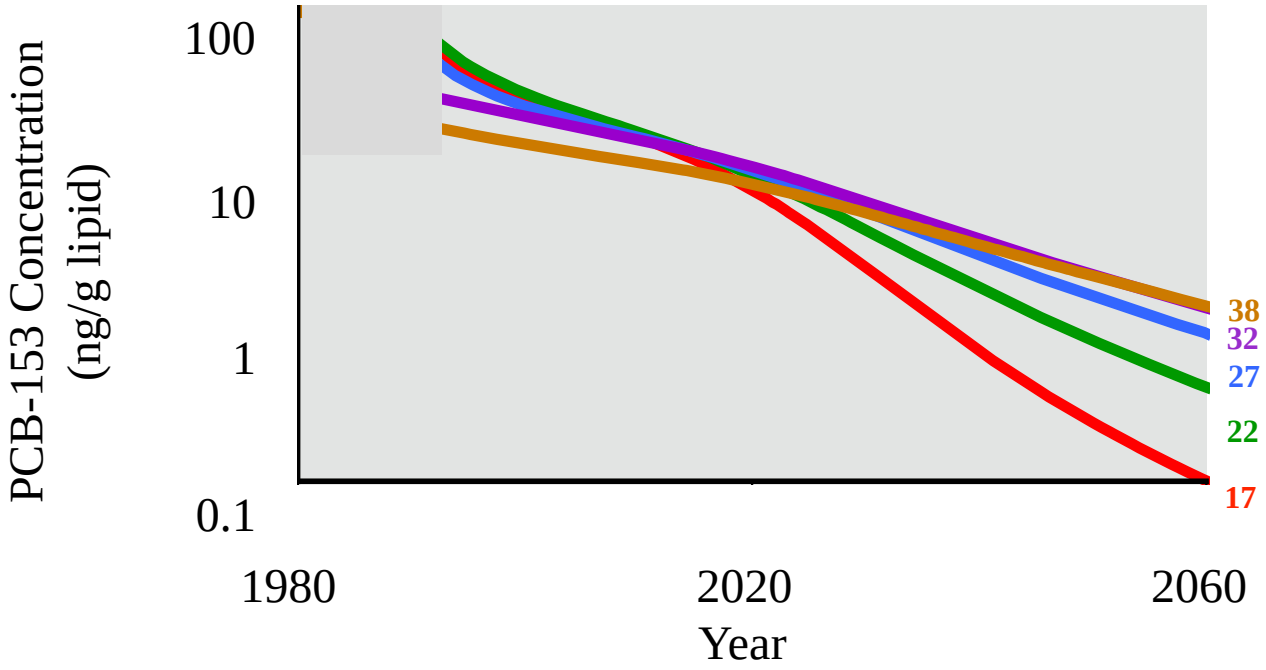
Would we expect slim or obese people to have higher PCB levels?

Growth curves/Lipid contents for males belonging to 5 BMI classes



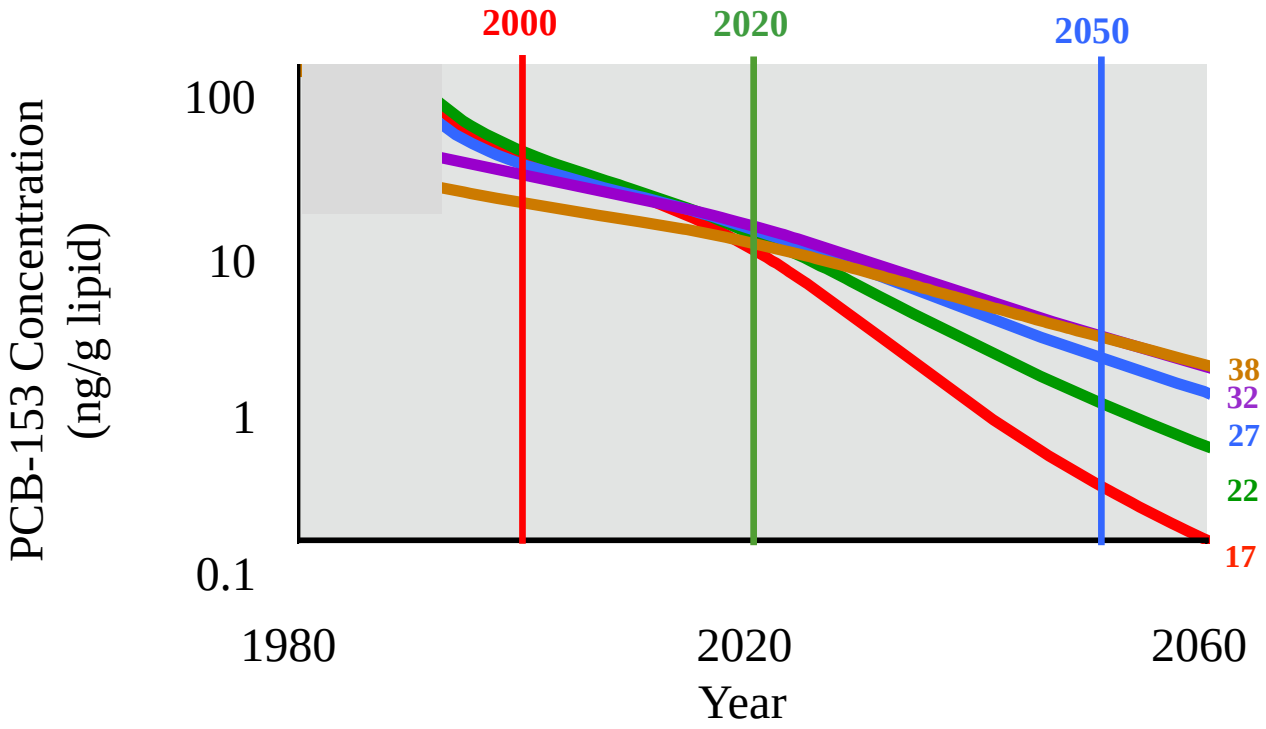
Would we expect slim or obese people to have higher PCB levels?

Longitudinal PCB concentration trends for individuals of the 1980s cohort (those born between 1975-1984) belonging to one of 5 BMI classes.



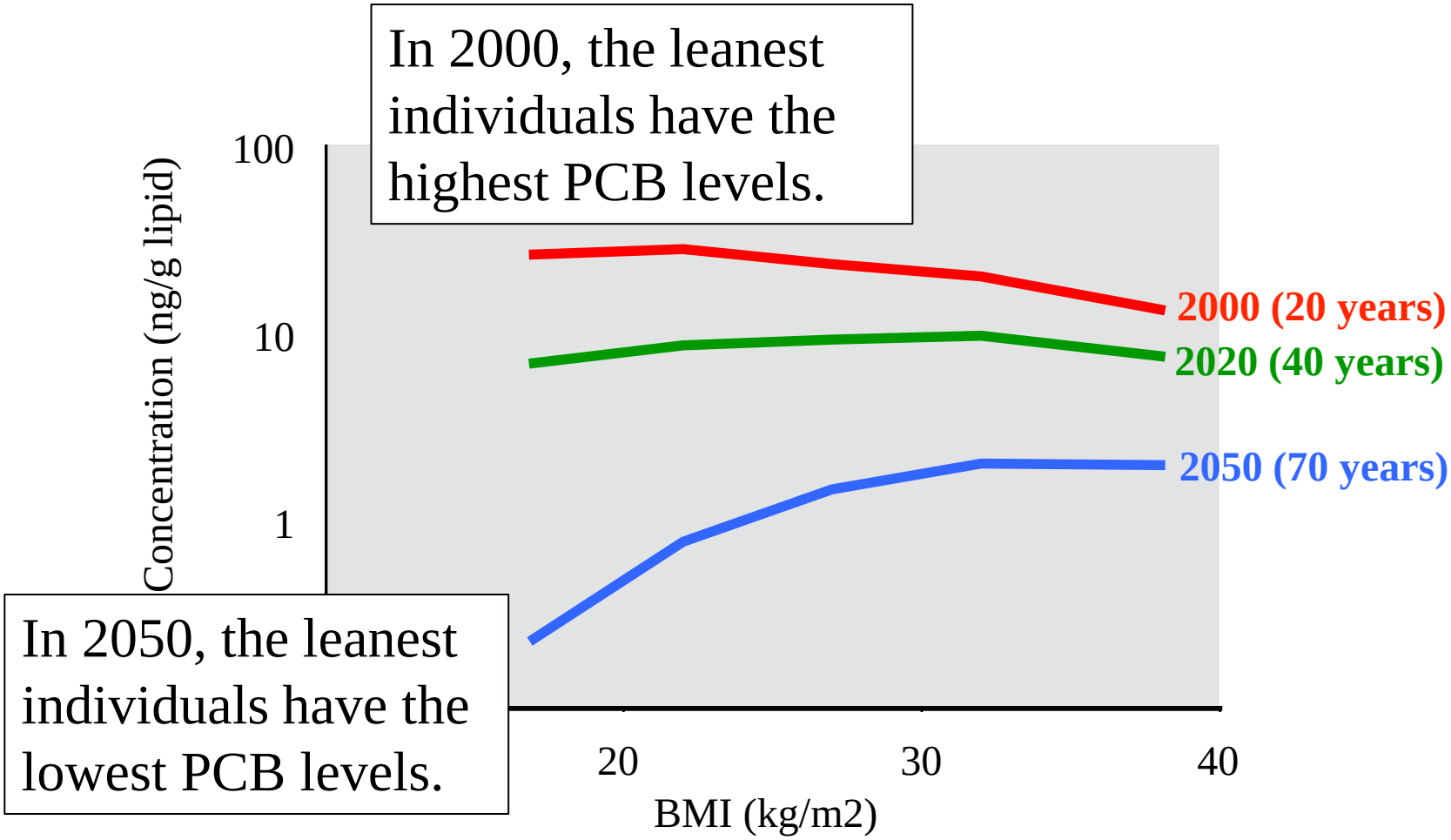
Would we expect slim or obese people to have higher PCB levels?

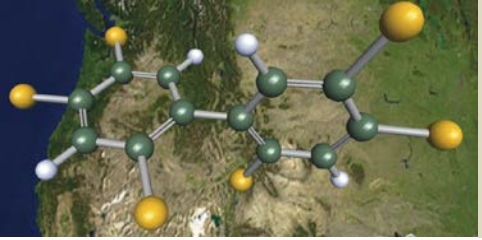
Each birth cohort is “sampled” repeatedly



Would we expect slim or obese people to have higher PCB levels?

to obtain cross-sectional PCB concentration – BMI relationships





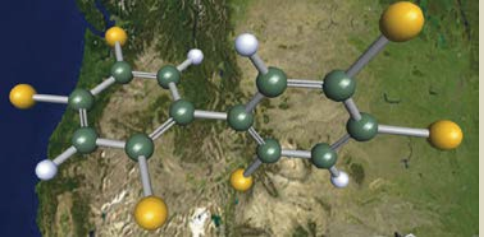
Would we expect slim or obese people to have higher PCB levels?

Within the same birth cohort, we can have PCB concentrations that increase, stay the same, or decrease with increasing BMI, depending on when the cohort is sampled.

Thermodynamics vs. kinetics

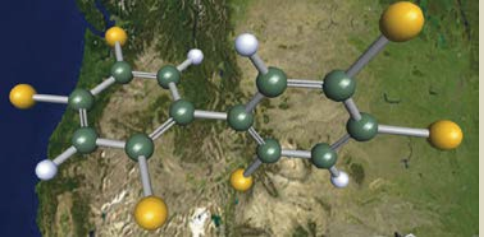
- Initially lipid-normalized PCB concentrations tend to be lower in obese than in lean individuals because of dilution in a larger volume of lipid
- Concentrations in all individuals decrease because of declining exposure
- Concentrations in obese individual decline slower than those in lean individuals (depuration half-lives range from 10 years for BMI17 to 14 years for BMI 38)

Wood et al. *Environ. Sci. Technol.* **2016**, *50*, 10,055-10,064



Can models provide insight?

- When repeatedly sampling a population for human biomonitoring, do temporal changes in dietary habits and body lipids confound time trends?

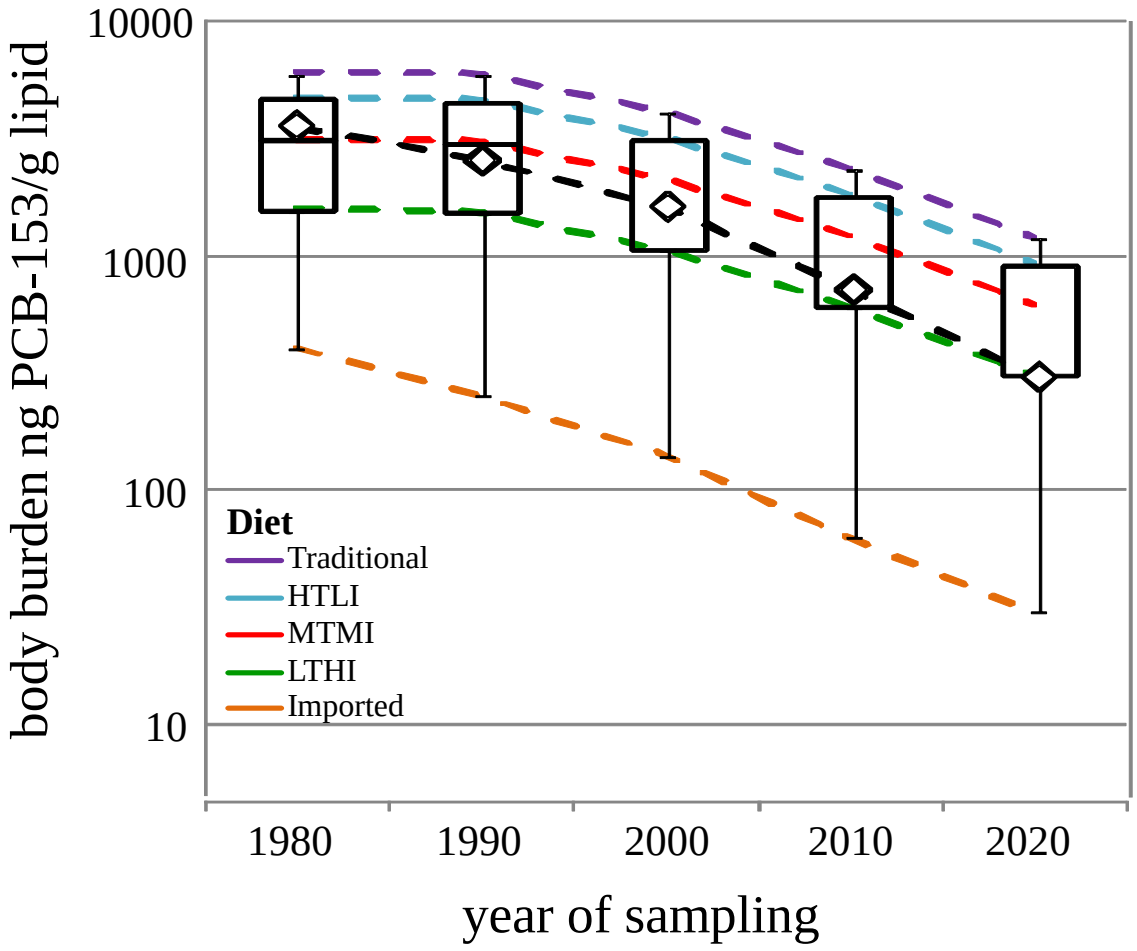


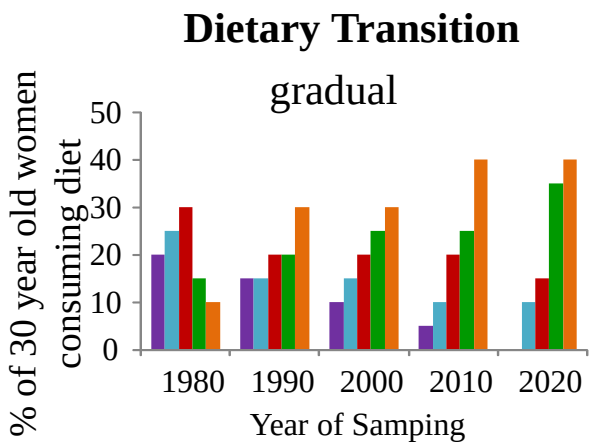
Do temporal changes in dietary habits confound time trends?

Example:
PCB levels in the Canadian Inuit population are decreasing over time.
Is this because of a decline in contamination of their environment or because younger generations eat more food imported from the South at the expense of traditional food?

Do temporal changes in dietary habits confound time trends?

time trends derived from repeated biomonitoring of 30 year-olds



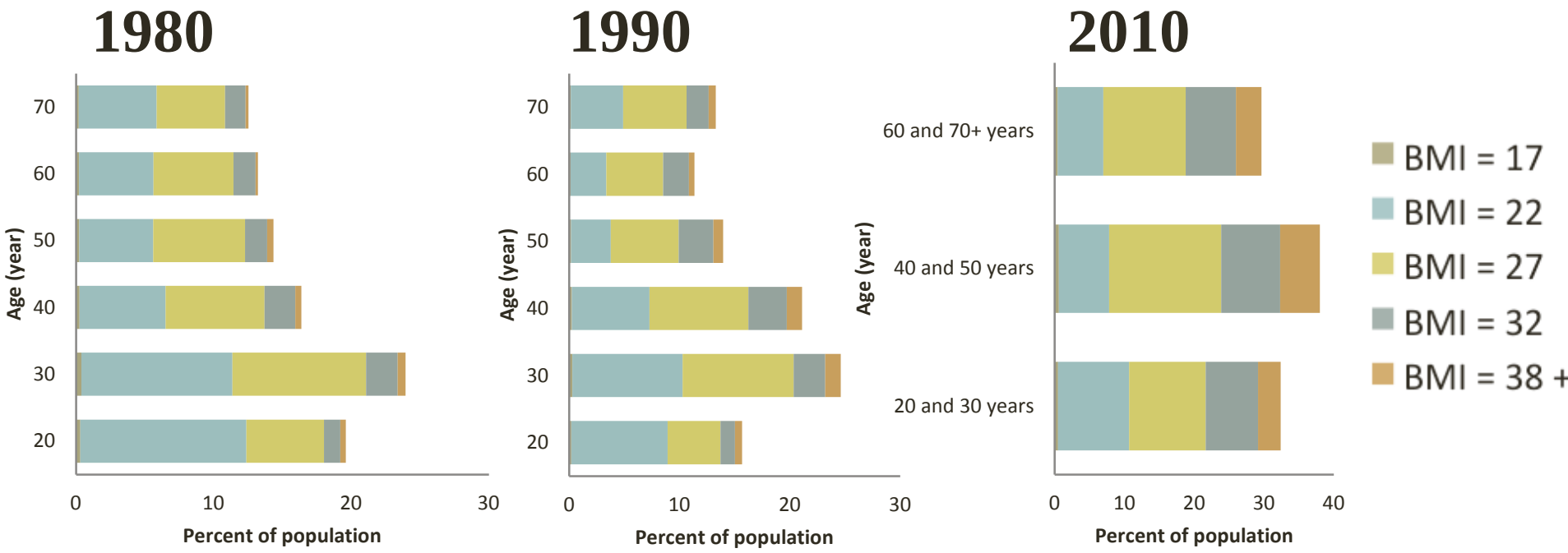


Each cohort is composed of individuals with a wide range of diets and it is the distribution of these diets which shifts increasingly towards more imported food items over time.

Quinn et al. *Environ. Int.* **2012**, *49*, 83–91

Do temporal changes in body lipids confound time trends?

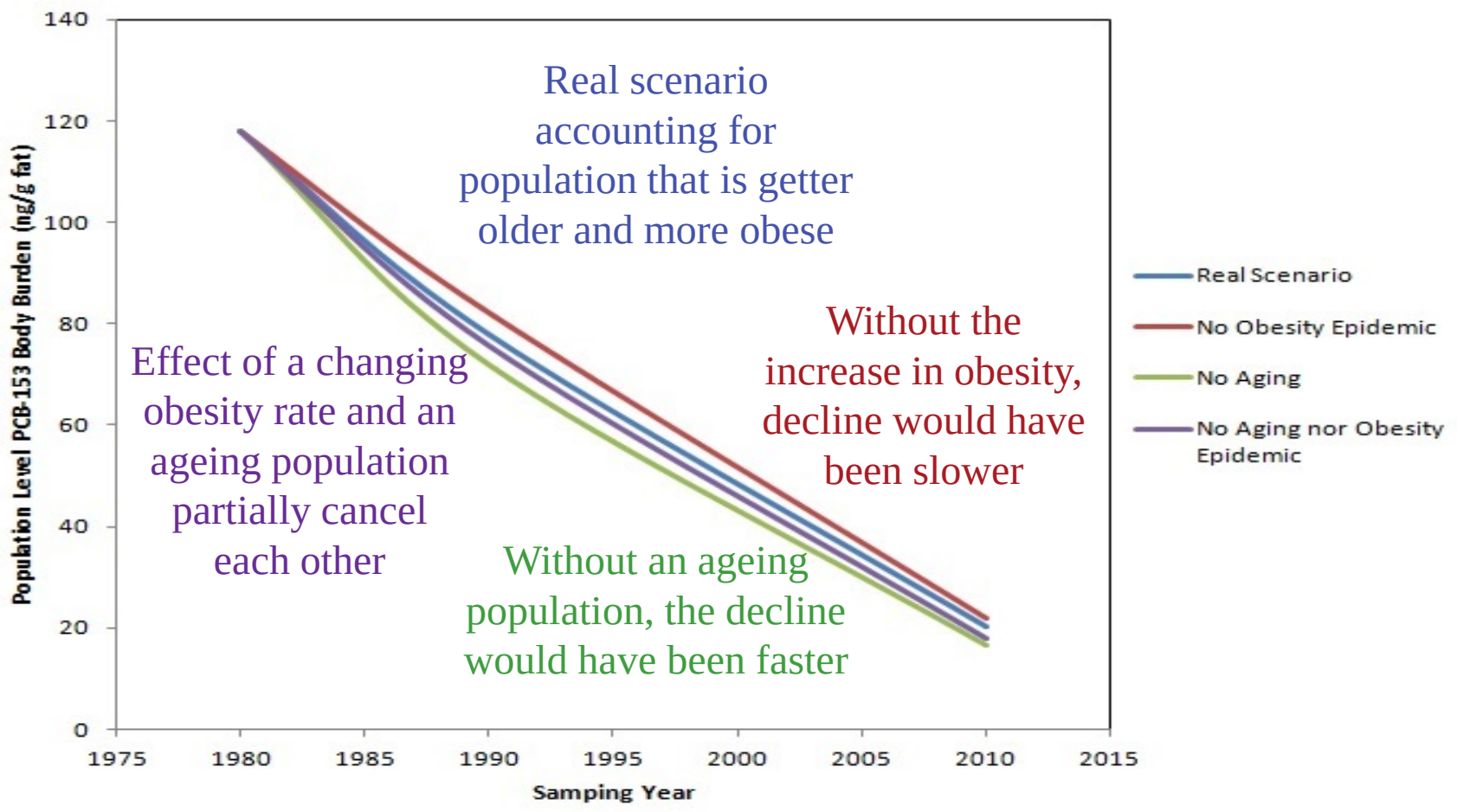
USA age and BMI distribution over time



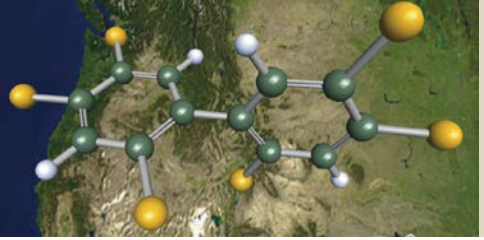
If you sample the US population repeatedly to derive time trends in PCB contamination, do you have to account for the changes in the population's BMI and age distribution?

Do temporal changes in body lipids confound time trends?

Population Average PCB Concentration



Wood et al. *Environ. Sci. Technol.* **2016**, *50*, 10,055-10,064



Can models provide insight?

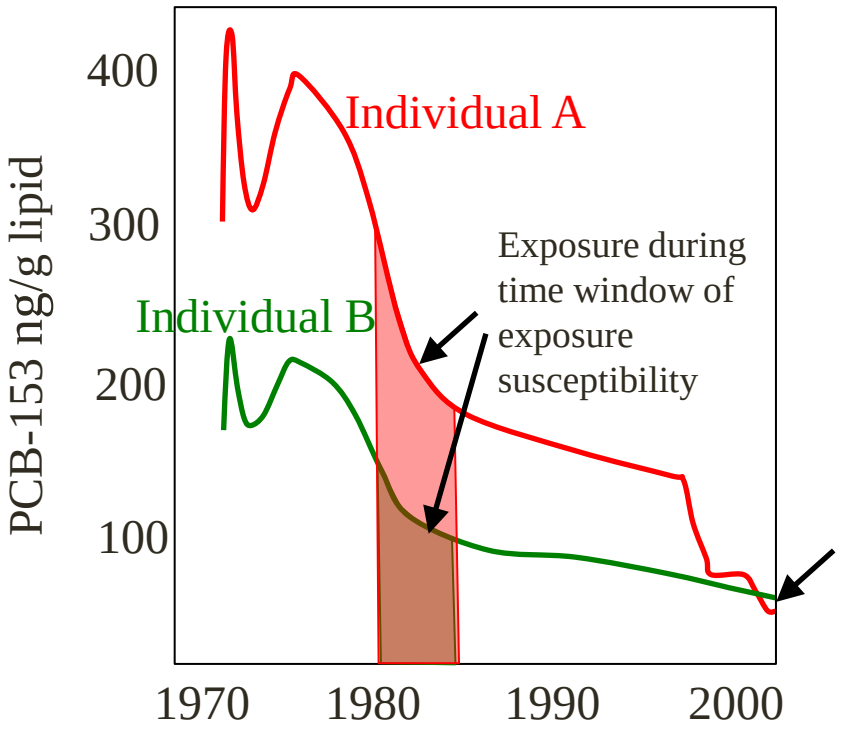
- When repeatedly sampling a population for human biomonitoring, do temporal changes in dietary habits and body lipids confound time trends?

Yes, the intergenerational dietary transition among the Inuit can be expected to influence population level time trends.

No, the obesity epidemic in the USA is not expected to strongly influence population level time trends, partly because it is countered by population aging.

Can models provide insight?

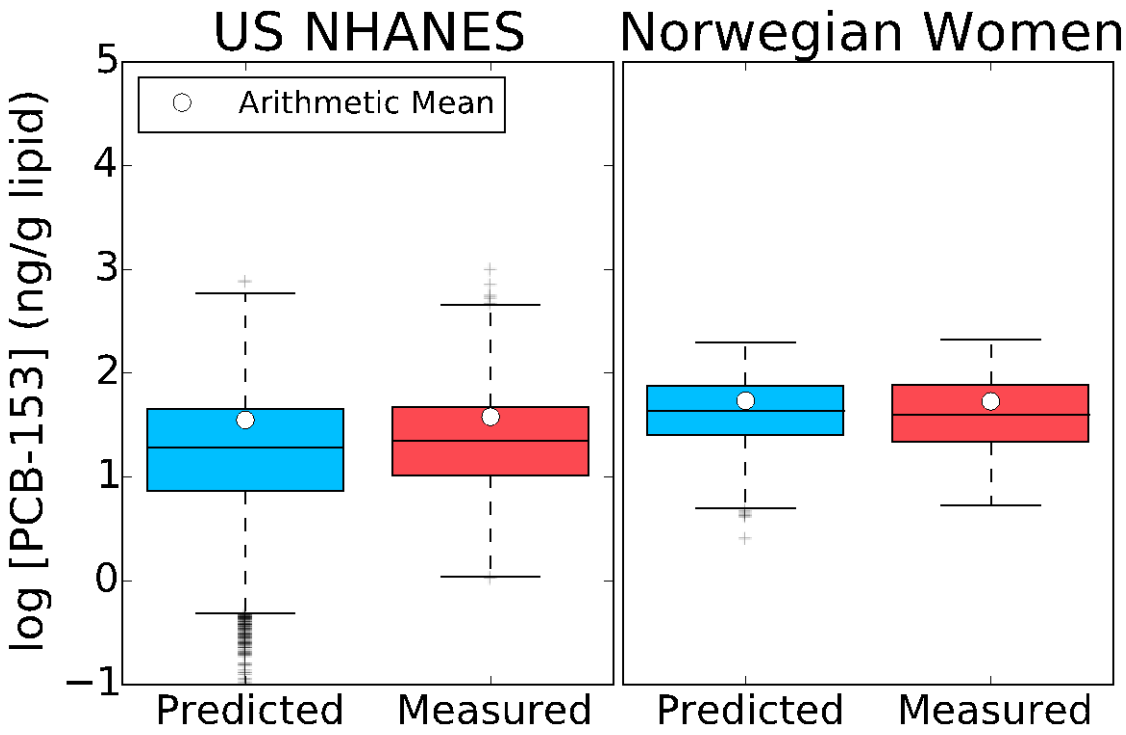
- Can we reconstruct past PCB exposure in individual humans?



Improving exposure characterization in epidemiological studies of contaminant health effects by reconstructing past exposure during age of susceptibility

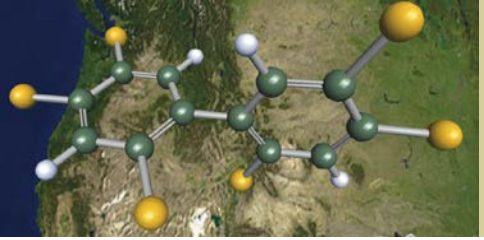
Rylander et al. *Env. Res.* **2015**, *142*, 365-373

Can we reconstruct past PCB exposure in individual humans?

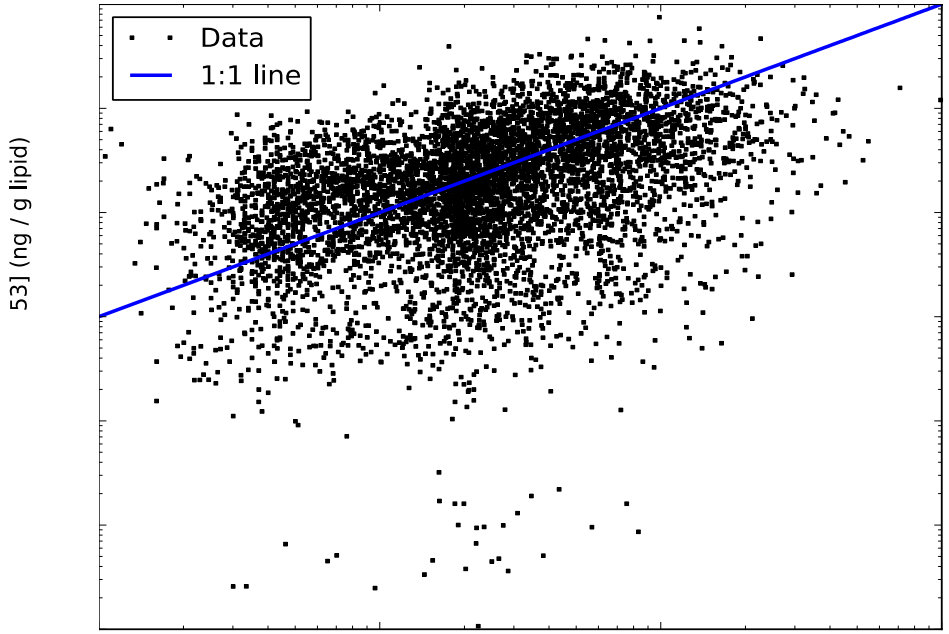


While we have succeeded in predicting the average and the variability in a populations' PCB exposure, …

Nøst et al. *Environ. Health Persp.* **2016**, *124*, 299-305
Wood et al. *Environ. Sci.: Processes Impacts* **2016**, *18*, 1157-1168



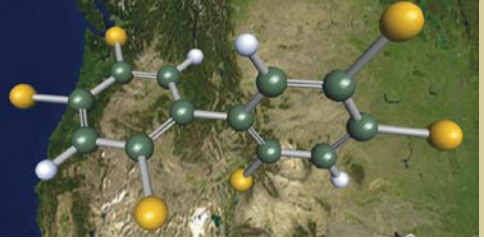
Can we reconstruct past PCB exposure in individual humans?



we have difficulty doing so at the level of the individual.

Weak link is getting reliable input on dietary composition at the level of the individual

Wood et al. *Environ. Sci.: Processes Impacts* **2016**, *18*, 1157-1168



Can models provide insight?

As long as the quality of the emission and property data of other organic contaminants does not match those of the PCBs, they will continue to serve an invaluable role in pushing the frontier in the field of environmental contaminant modelling

Acknowledgements

Cristina Quinn, Matt Binnington, Stephen Wood
James Armitage
Therese Nøst, Knut Breivik
Gertje Czub, Michael McLachlan

CLEAR Climate Change, Enviromental Contaminants and Reproductive Health

NSERC CRSNG

Canada Indigenous Affairs and Northern Development

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