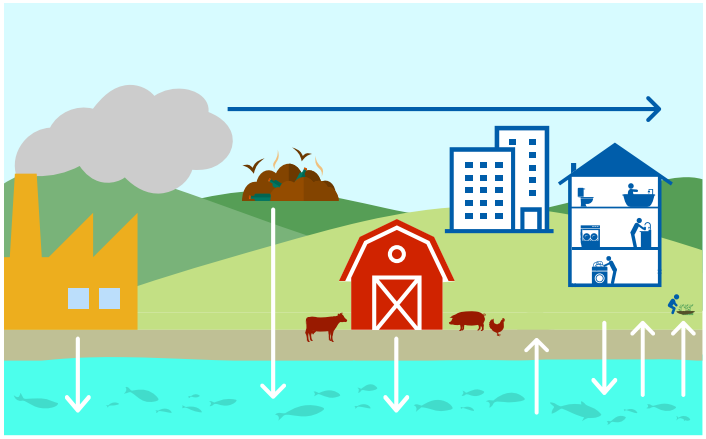
Simulation Science

ATSDR



Public health professionals and university researchers use the Agency for Toxic Substances and Disease Registry's (ATSDR) Simulation Science, or computer modeling, to learn how chemical exposure may affect health.

ATSDR collaborates with investigators at CDC and those outside the agency to understand the possible risks to human health when a person is exposed to toxic substances. When investigators enter the chemical/s they are interested in understanding into the computer program, it generates the information.

Simulation Science is a game changer because it ...

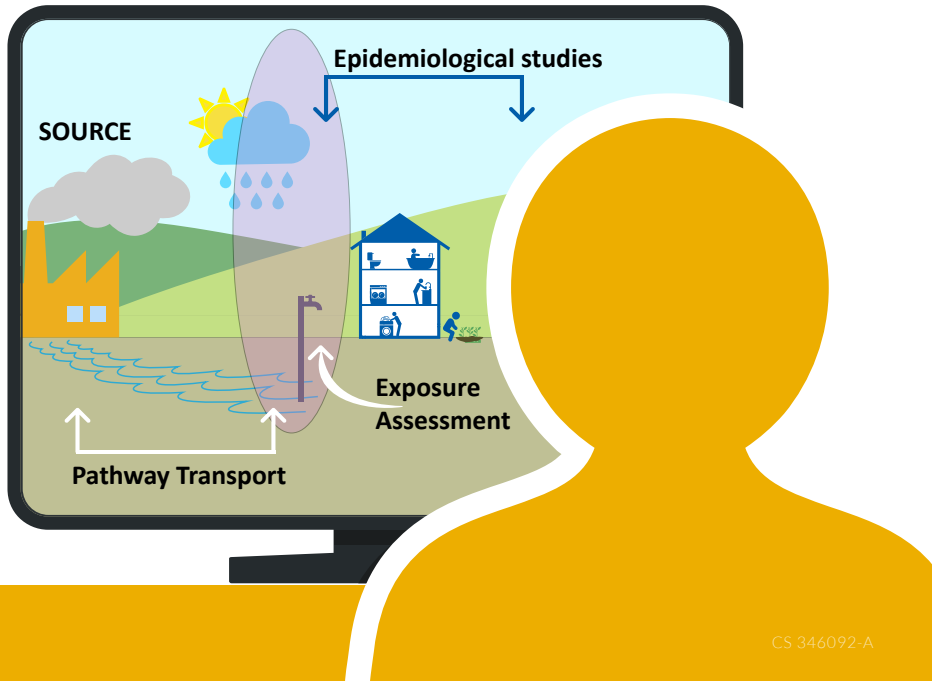
Requires neither human subjects nor lab animals, which saves resources and money.

Answers questions about human exposures in situations that haven't happened or that are difficult to recreate in a lab.

Quickly identifies health risks to thousands of hazardous substances, saving critical time in an emergency.

Computer modeling answers important questions.

- How does a chemical move and change in the environment?
- What is the estimated amount of chemicals in a person's body?
- What are the possible human health effects that are linked to a chemical?
- Is there any information about the health effects from chemical exposure that has been overlooked or is missing?



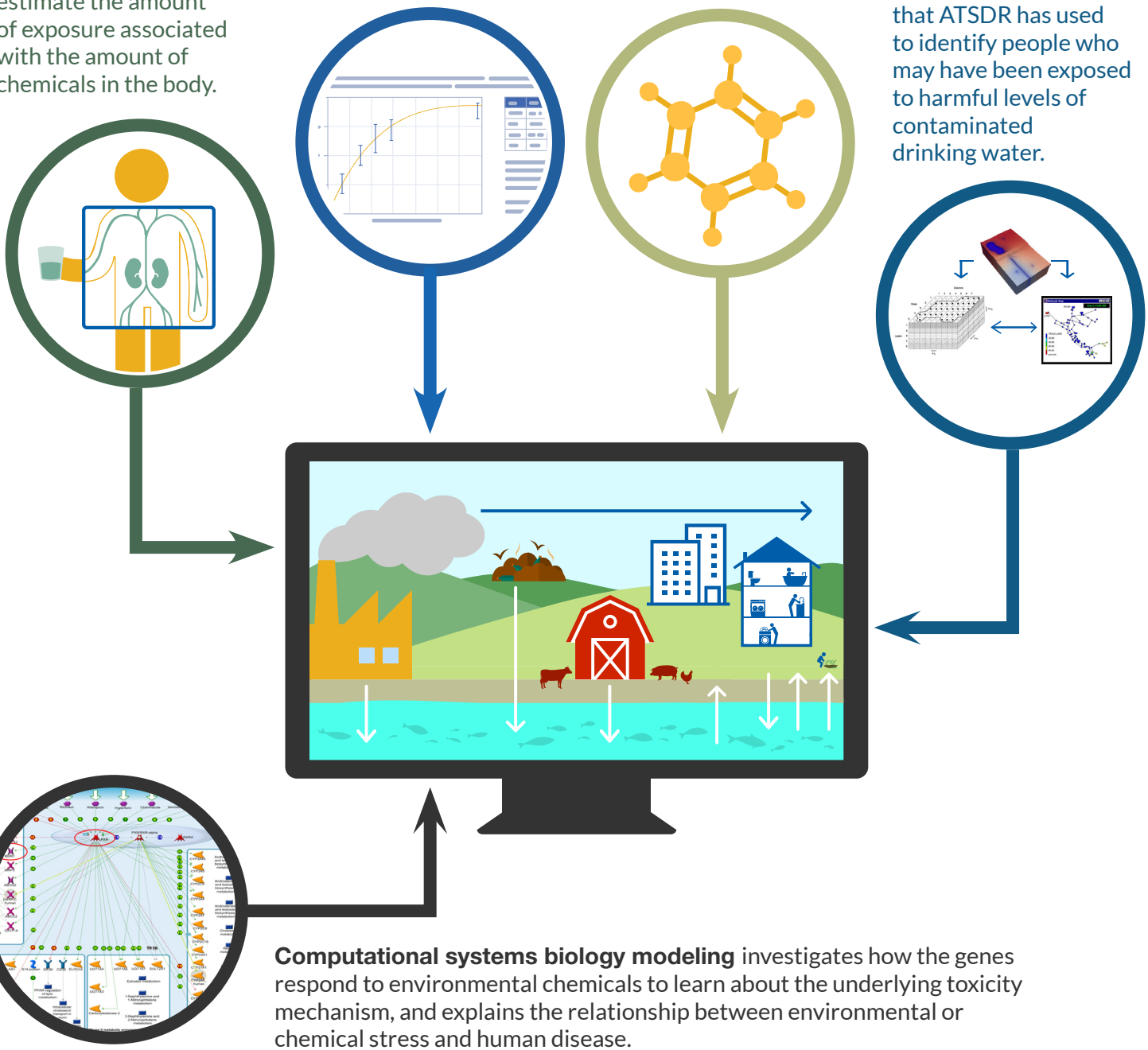
ATSDR's Simulation Science Section's four main computer modeling types

Physiologically based toxicokinetic (PBTK) models describe what happens when chemicals enter a person's body – which helps estimate the amount of exposure associated with the amount of chemicals in the body.

Benchmark dose models help determine whether a specific amount of a chemical may produce a certain harmful effect (like weight loss or growth of a tumor).

Structure-activity relationship (SAR) models help identify potential health effects of unknown or poorly understood substances by comparing them to those that have similar chemical structure and have been well-studied.

Fate and transport models predict how chemicals move in and transfer between air, soil, and water. Water models are a type of fate and transport model that ATSDR has used to identify people who may have been exposed to harmful levels of contaminated drinking water.



Computational systems biology modeling investigates how the genes respond to environmental chemicals to learn about the underlying toxicity mechanism, and explains the relationship between environmental or chemical stress and human disease.

If you're interested in collaborating with ATSDR's Simulation Science Section, or if you'd like to use computational modeling in your research project or initiative, contact Simulation Science Section Chief Patricia Ruiz at Patricia.Ruiz@cdc.gov