MS Program in Environmental and Green Chemistry at GWU

Prof. Jakub Kostal

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The Green Chemistry Education Webinar Series

The Green Chemistry Commitment
TRANSFORMING CHEMISTRY EDUCATION
Assessing the need

- Sustainability and ‘Green’ Jobs are a growing industry

Source: BLS
Program description

• 30-credit hour MS program
• 5 core focus areas: energy, environmental analytical chemistry, air/water chemistry, green chemistry processing and green toxicology
• Interdisciplinary, in close collaboration with: GWU School of Public Health, School of Public Policy and Administration and School of Engineering and Applied Sciences
• Highly customizable curriculum to suit personal needs and goals
• Housed by Chemistry department
Core courses: 1. Energy and the Environment

• Fundamentals of energy conversion
• Fossil fuel, hydrogen, nuclear and renewable resources systems
• Fuel reforming, hydrogen and synthetic fuel production, fuel cells and batteries, combustion of fossil and bio-derived fuels, hybrids, catalysis, supercritical and combined cycles, photovoltaics, etc.
• Energy storage and transmission
• Source utilization and fuel life cycle analysis

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2. Environmental analytical chemistry

• Advanced modern analytical methodology
• Analytical instrumentation, remote measurements, trace atmospheric constituents, uncertainty analysis, pollutants in air/water/soil and biota, heavy metals and radionuclides
• Emphasis on priority pollutants according to US regulatory agencies

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3. Environmental chemistry of water, air and soil

- Behavior, movement and impact of chemicals in air, water and soil
- Chemistry of environmentally important cycles
  - Human factors: acid raid, sewage treatment, ozone destruction, climate change, air pollution and eutrophication

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4. Green chemistry processing

- Design principles for greener technologies
- Challenges and trade-offs in shifting production toward renewable technologies
- Social and technical factors affecting adoption of ‘greener’ solutions
- Focus on real-world case studies

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5. Green Toxicology

• Basic tools and paradigms of predictive toxicology
  medicinal chemistry principles
  computational chemistry/biology methods
  QSARs, expert systems, read-across
  spectroscopic tools

• Focus on strategies for safer chemical design

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Capstone project

• A group-based project in partnership with an external partner/client or a participating Chemistry Department faculty member.

**External partners/clients for capstone projects**
- **Government agencies**: e.g. EPA, DoE, FDA, NIH, NIEHS;
- **NGOs**: e.g. Environmental Defense Fund; Environmental Working Group; Natural Resources, Advancing Green Chemistry, Clean Production Action,
  BizNGO, Lowell Center for Sustainable Production;
- **Private sector organizations**: e.g. Seventh Generation, Dow,
  DuPont, ToxServices, SciVera
- **Industry groups/ roundtables**: e.g. GC3 Council, American Chemical Society, Institute for Green Chemistry
- **Academic partners**: e.g. Berkeley Center for Green Chemistry, Yale Center for Green Chemistry, GreenCentre Canada.
CHEM 6283
Chemical Toxicology and Rational Design of Safer Chemicals
Spring 2017

• Class materials:


  Cradle to Cradle: Remaking the Way We Make Things, M. Braungart (2002)


  Cronin, M. T. D. and Madden, J. C. (Editors). In silico Toxicology. Principles and Applications. RSC Publishing 2010
Learning Objectives

• Understand toxicological impact of the chemical industry in a historical context
• Use toxicological data for hazard assessment
• Use mechanistic toxicology to identify relevant structural features in chemicals and link them to biological effects
• Understand the tenets of risk assessment (hazard vs. exposure) and life-cycle analysis
• Use computational tools and metrics to evaluate and compare hazard profiles
• Design chemicals that are ‘safe’ with respect to several toxic endpoints
Course description:

1. Chemical industry and case studies of chemicals of concern
   a. BPA
   b. Phthalates
   c. Flame retardants

2. Mechanistic toxicology: Modes of action of chemical classes
   a. Connecting reactivity *in chimico* and *in vivo* with focus on electrophilic chemicals
   b. Alkanes, alkenes, alkynes
   c. Epoxides
   d. Benzene
   e. Polyaromatic hydrocarbons
   f. Polybrominated aromatics

3. Toxicology for chemists
   a. General principles: dose response curves, statistical methods
   b. Mechanistic toxicology – toxicokinetics and toxicodynamics
   c. Toxicogenomics
   d. Absorption, Distribution, Metabolism and Excretion
   e. Ecotoxicology

4. Types of toxicological data
   a. Overview of types of toxicological testing - models, tools, terminology and limitation
   b. Acute vs chronic
   c. Endpoints
      i. *In vivo* assays – fish
      ii. *In vivo* assays – small mammals
         - Assay-tox models - (including what is an assay)
   a. Data sources and data quality
   b. Overview of non-animal testing - what is an assay?
   c. In vitro methods
   d. High throughput screening
   e. TOXCAST and other data sources
5. Risk Assessments vs Alternatives Assessment
   a. Hazard vs exposure
   b. What is a risk assessment?
   c. Steps in carrying out a risk assessment
   d. Overview of an AA and its components
   e. Define a chemical hazard assessment
   f. Data gaps exist for existing chemicals

6. Modeling and Predicting Toxicity
   a. Quantitative Structure Activity (Toxicity) Relationships
   b. Statistical methods used in QSAR and QSTR analyses
   c. Computational methods used to predict toxicity
   d. Automated Rule Induction Systems
   e. Knowledge-Based Expert Systems
   f. Rea-across approaches

7. Regulation and Policy
   a. EPA and TOSCA, EU and REACH
   b. Pesticides
   c. Chemicals in food and cosmetics

8. Global Hazards
   a. Review of atmospheric chemistry: aerosols, greenhouse gases, climate change
   b. Introduction to aquatic chemistry
   c. Terrestrial environmental concerns
      i. Persistence
      ii. Soil pollution

9. Chemicals in water
   a. Organic chemicals and pharmaceuticals in municipal water and environment
   b. Biodegradation of pharmaceuticals
   c. Catalytic systems for degradation of organics
   d. Alternative methods for extraction: reverse osmosis

10. “Green” nanotechnology
    a. Modes of action of nanoparticles
    b. Evidence of toxicity
    c. Designing a safer nanoparticle

11. Principles for designing safer chemicals
    a. Design guidelines for minimizing bioavailability
    b. Design guidelines for minimizing mutagenicity
    c. Design guidelines for minimizing aquatic toxicity

12. Designing for biodegradability
    a. Biodegradation by functional group
    b. Design guidelines
    c. Cradle to cradle
Case Study

Fathead minnow LC$_{50}$, 96-h assay
U.S. E.P.A.
555 chemicals

**“safer chemical space”:** $\log D_{o/w} < 1.7$, $\Delta E > 6$ eV

Safer chemical design guidelines:
$\Delta E = 6.62$ eV and $\log D = 5.09 \rightarrow$ not SAFE to aquatic species

LC$_{50}$ (Fathead minnow, 96hr): 0.87 mg/L
Suitable alternatives?

TPP:
Suitable alternatives with similar functionality?

TPP:

- ΔE = 6.6 eV, logD = 5.1
- ΔE = 6.4 eV, logD = 5.6
- ΔE = 6.5 eV, logD = 6.1
- LC50: 0.25 (High tox)
  - ΔE = 6.4 eV, logD = 6.6

- ΔE = 8.6 eV, logD = -0.11
- ΔE = 8.8 eV, logD = 1.2
- LC50: 350 (low/no tox)
- ΔE = 8.5 eV, logD = 0.76
- ΔE = 8.5 eV, logD = -0.52
Designing safer OP compounds for specific endpoints:

![Diagram showing box plots for different endpoints: Narcosis, ACHE Inhibition, CNS Seizure, Electrophilic, Neurodepressants, Other, Resp. block, Uncoupled oxid. phos.](image)

- Narcosis: 
- ACHE Inhibition: 
- CNS Seizure: 
- Electrophilic: 
- Neurodepressants: 
- Other: 
- Resp. block: 
- Uncoupled oxid. phos.:
Active site of AChE: Binding affinity of OPs
Admission requirements

- GRE scores
- bachelor’s degree in science or engineering (GPA of 3.0 or above)

At minimum, candidates must have completed:
- Two semesters of general chemistry
- Two semesters of organic or inorganic chemistry
- One semester of quantitative and/or instrumental analysis (recommended)

Supporting Documents Required:
- Official transcripts from all post-secondary institutions attended
- 2 letters of recommendation
- Resume/CV
- Personal Statement

For International students
- Minimum TOEFL scores: 85
- Minimum IELTS score: 6.5
Contact Info

Department website (application link):
https://chemistry.columbian.gwu.edu/ms-environmental-and-green-chemistry

(Application deadline April 1 – Fall semester, October 15 – Spring semester)

Financial Aid:
https://chemistry.columbian.gwu.edu/graduate-student-admissions-and-financial-aid

Further inquiries:
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