CENTER FOR GREEN CHEMISTRY & GREEN ENGINEERING AT YALE

Using a computer game to introduce green chemistry and safer chemical design concepts into an undergraduate curriculum

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Education is undergoing transformation

- Conventional teaching is frequently static and fails to develop skills such as critical thinking and problem solving.
- Modern curriculum can retain students at a higher rate.
- Studies have advocated for increasing interdisciplinary content and improving the relevance for high school and undergraduate students.
- Videos, simulations and hands-on activities allow students to make more connections between the scientific topics.

Journal of Science Education and Technology 2009, 18, (4), 305-320.

"…digital game-based learning has been recognized as a promising approach for motivating students to learn "

Kiili, K. (2007). Foundation for problem-based gaming. British Journal of Educational Technology, 38(3), 394–404.

Education and computer games

Is this a new trend?

Where in the world is Carmen Sandiego? ‘85

Educational mystery game where player uses the knowledge of geography, history and world cultures to track the thief.

As more thieves are arrested, the player rises in the ranks and cases become more difficult.

Where in the USA is Carmen Sandiego? ‘86
Where in the Europe is Carmen Sandiego? ’88
Where in the Time is Carmen Sandiego? ’89
Where in the Space is Carmen Sandiego? ‘93

Educational games now

- Emerging are *epistemic games* (virtual internships) which allow students to role-play professionals (including architects, journalists, urban planners, and engineers).
  - Exposure to practices, design process, experience, team work, minimal financial resources

- Virtual internships allow solving complex science, technology, engineering and math (STEM) problems.

- However the majority of educational games are intended for K-12

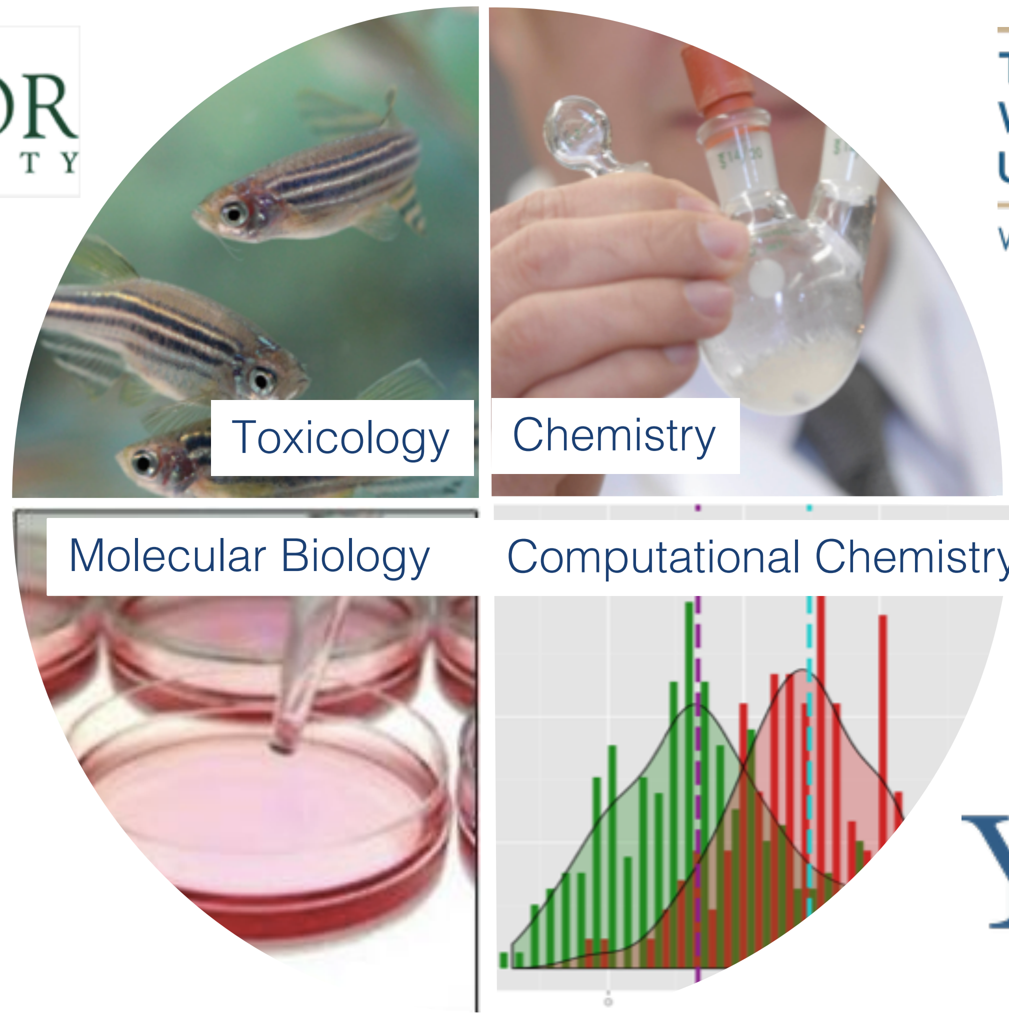
MoDRN

Molecular Design Research Network

BAYLOR UNIVERSITY 1845

THE GEORGE WASHINGTON UNIVERSITY

WASHINGTON, DC



UNIVERSITY of WASHINGTON

Yale

Molecular Design Research Network (MoDRN)

Our educational approach

Novel research in chemistry and toxicology (scientific literature, MoDRN's research)

Scientifically rigorous, easily accessible educational materials which:

- Engage students in safer chemical design of the next generation molecules
- Allow seamless integration in the chemistry, biology or environmental science curriculum.

Green Chemistry & Safer Chemical Design Game

Main objectives

- Develop an educational game which can be used by non-major undergraduate students to make connection between physiochemical properties and health.

- Disseminate 4th Principle of Green Chemistry

Green Chemistry & Safer Chemical Design Game

- Unique activity which incorporates systems thinking into the product design.
- It simulates scenarios to model decision making process used by professionals to develop a new chemical product.
- Players complete multiple stages of product design with respect to environmental and human impacts, and performance.

The team

- Research team Center for Green Chemistry & Green Engineering
- MoDRN consortium of toxicologists, molecular biologists and environmental scientists
- Center for Teaching and Learning at Yale
- Yale ITS (2 Teams!)
- Yale undergraduates
- Aptara – online gaming expert

Steps in building the game

1. Define which chemistry and toxicology concepts do we want to highlight in the game.
2. Decide what other life-cycle concepts should be included.
3. Define metrics, boundaries, data sources, IT requirements.
4. Develop a framework which includes scientific and educational components and links them together.
5. Build a ‘wireframe’ (storyline, avatars, graphics).
6. Develop scientifically accurate language which supports a wireframe (tasks, tips, feedback).
7. Test the game logic.
8. Engage the group and receive feedback.

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Define which chemistry and toxicology concepts we want to highlight in the game.

- ADME - Absorption, Distribution, Metabolism and Elimination.
- Differences/similarities between human and aquatic toxicity.
- Physicochemical parameters like molecular weight, log P and physical state and their role in ADME. Limiting bioavailability and enhancing DME.
- The role and the structure of product, in this case a surfactant.

Decide what other life-cycle concepts should be included

- Chemical performance: what is detergent's cleaning ability?

Define metrics, boundaries, data sources, IT requirements

- Use parameters and their preferred/not preferred ranges that limit or enhance toxicity described in peer reviewed literature and MoDRN's work.

- Provide simple explanations of the complex toxicology/biochemistry terms

e.g.: Log P definition = Log P is a measure of lipid solubility (how well the chemical dissolves in fat and passes through cell membranes).

Rather than LogP = **partition-coefficient** is the ratio of concentrations of a compound in a mixture of two immiscible phases (water and octanol) at equilibrium.

$$\log\ P_{\text{oct/wat}} = \log\left(\frac{[\text{solute}]_{\text{octanol}}^{\text{un-ionized}}}{[\text{solute}]_{\text{water}}^{\text{un-ionized}}}\right)$$

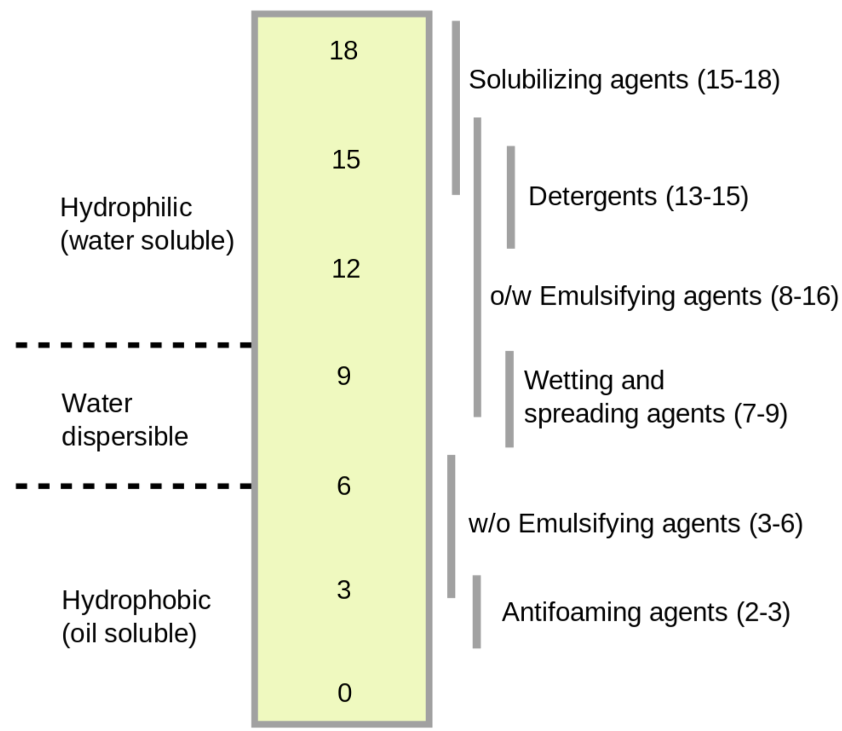
Define metrics, boundaries, data sources, IT requirements

Performance of the detergent metrics = HLB value

HLB hydrophilic-lipophilic balance is a measure of the degree to which surfactant is hydrophilic or lipophilic.

It's value depends on Log P and the presence of the functional groups (esters, aldehydes, alcohols)

Is expressed on the scale 0-18



Goal & Gameplay

Player has to come up with the optimal detergent which:

- Is benign by design (does not cause human/aquatic toxicity)
  - LEVEL 1: Has a limited absorption through membranes (limited bioavailability)
  - LEVEL 2: If absorbed, it has a reduced movement through the body (distribution), increased deactivation rate (metabolism) and accelerated removal (elimination)
  - Biodegrades in the environment
- Has an optimal cleaning performance

Notes:
One detergent is optimized throughout the Level – property selection carries from one challenge to another

Detergent design is based on properties not a molecular structure

LEVEL 1

GOAL

HUMAN TOXICITY
- Skin absorption
- Lung absorption
- Intestine absorption

AQUATIC TOXICITY
- Avoiding toxicity

PERFORMANCE

LEVEL 2

GOAL

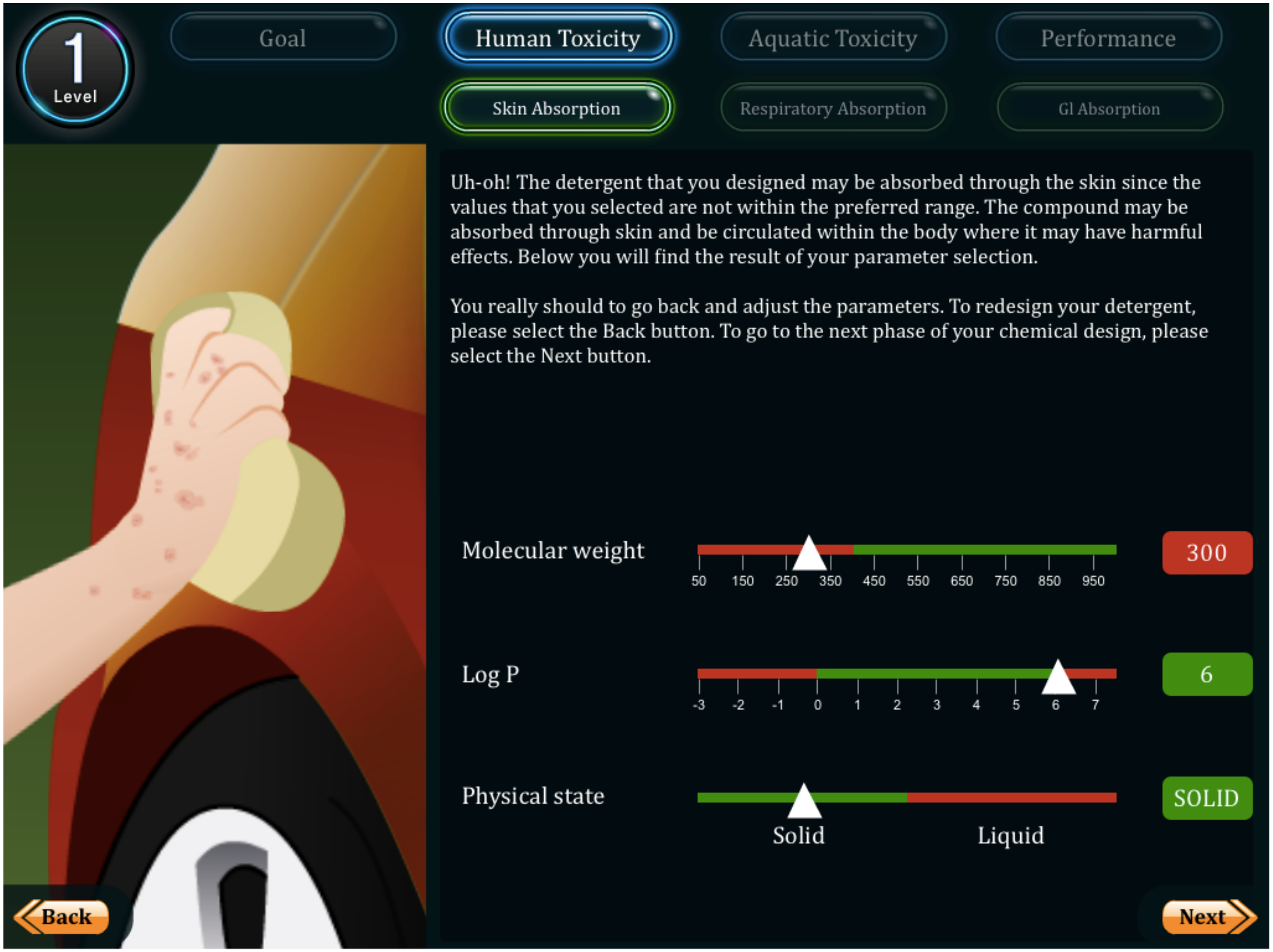
HUMAN TOXICITY
- Distribution
- Metabolism
- Elimination

AQUATIC TOXICITY
- Biodegradation

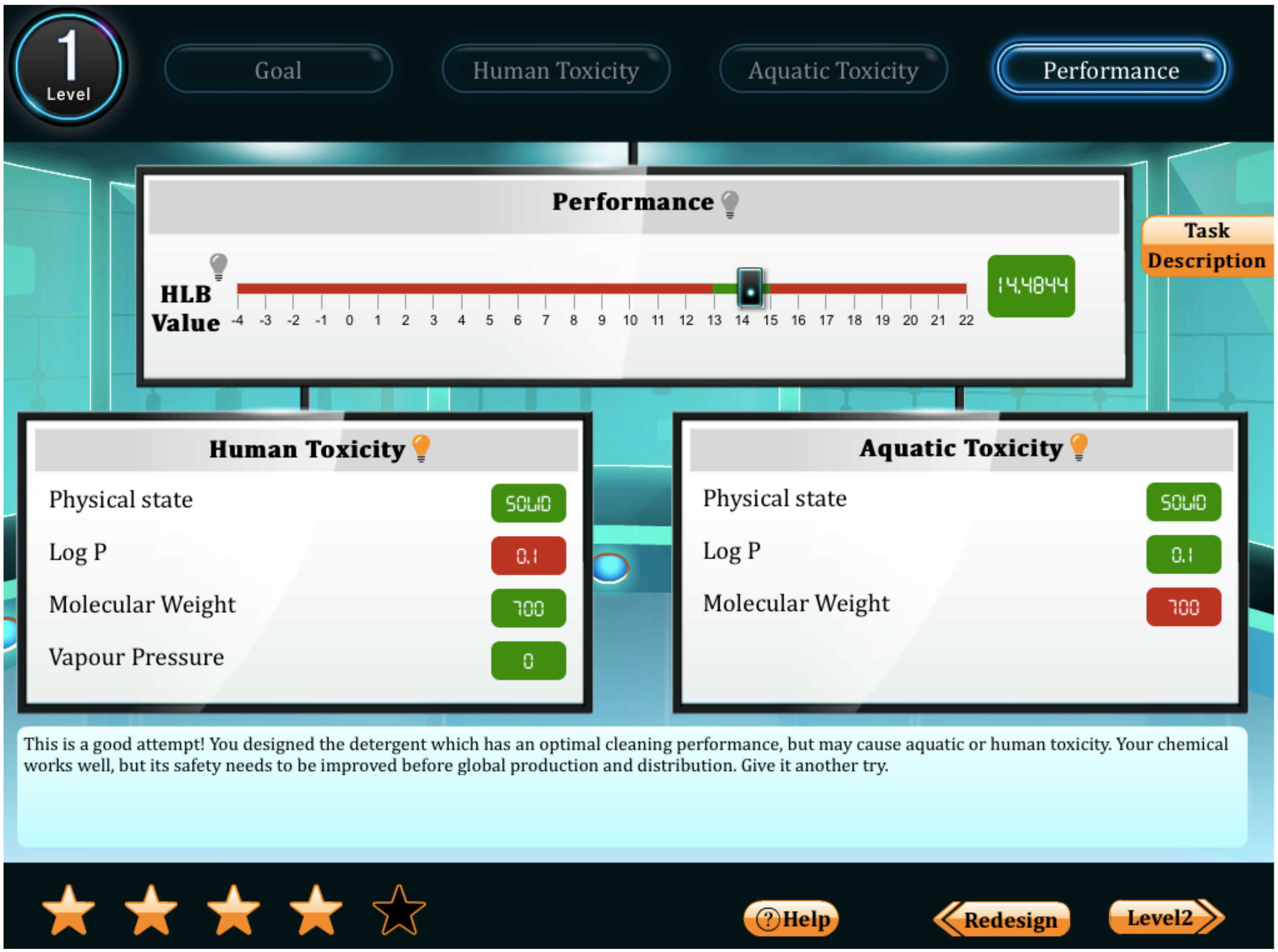
PERFORMANCE

Other features that enhance learning experience: Tips for parameter selection

Other features that enhance learning experience: Instant feedback & suggestions for improvements



At the end:
"stars" and feedback for a successful design



Next steps

- Work with a pilot group of students and faculty to conduct a beta testing
- Release the game to the public
- Interested? Please reach out!

Acknowledgements

- Center for Green Chemistry & Engineering
  - Paul Anastas, Philip Coish, the entire Anastas group
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- Center for Teaching and Learning at Yale
- Yale ITS
- Aptara

Yale Center for Teaching and Learning

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