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v Ljubljani

Fakulteta *za kemijo*  
*in kemijsko tehnologijo*

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**VABILO NA PREDAVANJE  
V OKVIRU DOKTORSKEGA ŠTUDIJA  
KEMIJSKE ZNANOSTI**

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z naslovom:

**Assessing the World Energy Crisis  
Equation from Mathematical Modeling**

**v sredo, 14. decembra 2016 ob 15:00 uri**  
v predavalnici 1 v 1. nadstropju Fakultete  
za kemijo in kemijsko tehnologijo, Večna pot 113

*Vljudno vabljeni!*

**Abstract:**

Mathematical models are being used almost everywhere: to engineer the bus you took this morning to go to your office, to manage trains traffic, to distribute energy in an efficient way within your country, to perform statistics on who will be the next president of France or to forecast the weather on next December 14, 2016, date in which this lecture will take place. Surprisingly, mathematics, supported on a combination of axioms and theorems, and crystallized in the form of algebraic and differential equations, generally works quite well, and has catalyzed many technological progresses in the last two centuries. Therefore, it will be legitimate to ask ourselves if mathematical models are simple and imperfect representations of real events, or if, in contrary, the real events are themselves made of mathematics. This dichotomy, which can sound outmoded, is seriously considered again by modern epistemologists and physicists in view of recent findings in modern physics.

First, this lecture will provide arguments, from experimental facts, supporting these two different visions. Then, the lecture will bring a review on the practical implications of using mathematics to solve one of the most challenging equations the humanity is facing today: the energy demand as function of the available energy resources, population raise and climate change. More specifically, the lecture will illustrate success stories on the use of mathematical models to design and optimize the next generation of electrochemical devices for energy storage and conversion, such as fuel cells and batteries. Recent progresses on the use of multi-paradigm/multi-scale computational methods and machine learning algorithms to perform *in silico* experimentation and to discover materials and operation conditions will be presented. The potentialities of combining these approaches with a new generation of data visualization tools based on immersive Virtual Reality, will be discussed. Finally, methodological challenges will be described through keywords such as data management, storage and interoperability and reusability.