Is Experimentation More Intuitive?

R Venkataraghavan
Unilever R&D Bangalore

Keynote Address at the COMSOL Conference, Bangalore, November 2011

About Unilever, Unilever R&D

People know us by our brands

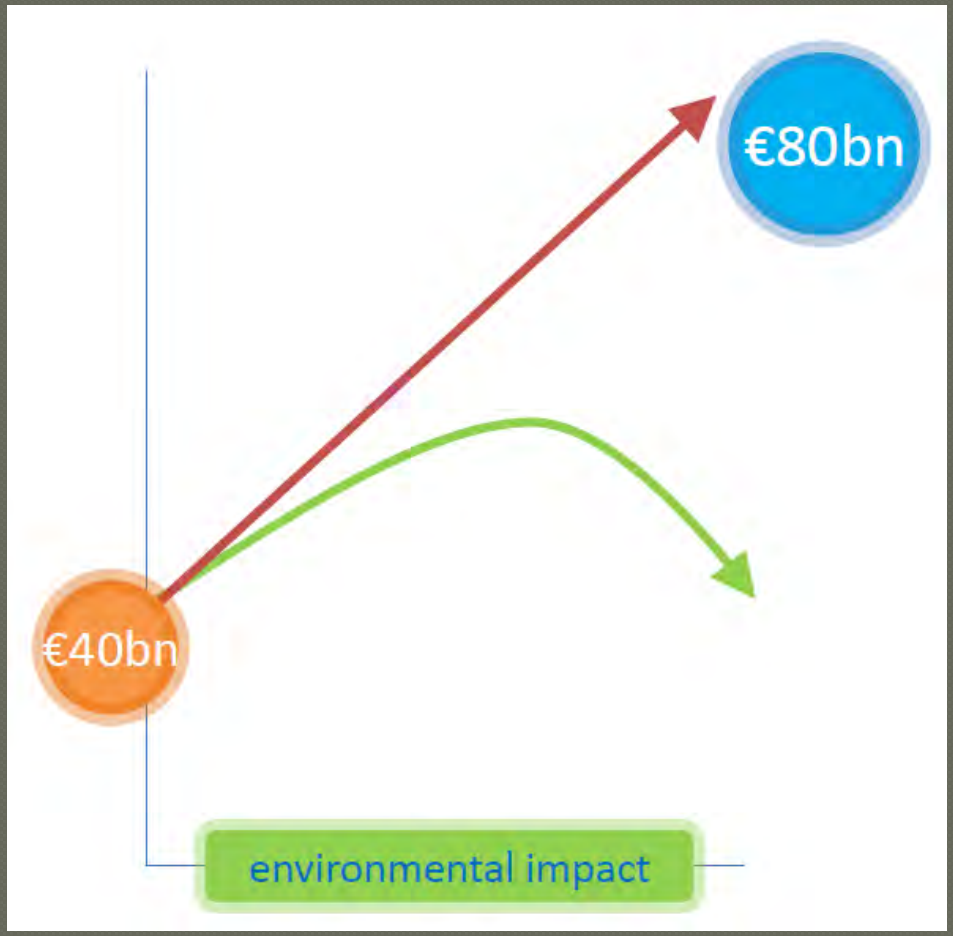
Compass: Our Vision

We work to create a better future every day.

We help people feel good, look good and get more out of life with brands and services that are good for them and good for others.

We will inspire people to take small, everyday actions that can add up to a big difference for the world.

We will develop new ways of doing business that will allow us to double the size of our company whilst reducing our environmental impact.



One Unilever R&D

4D model of the new organisation

Prioritise in Define

Breakthroughs From **Discover**

Brilliance In Product **Design**

Fast, Large Scale **Deploy**

Differentiating and Transforming
Critical Functional Capabilities

SAFETY

CLINICALS

OPEN INNOVATION

REGULATORY AFFAIRS

PATENTS

IT FOR R&D

Discover Focussed on Six Key Labs

Colworth

Vlaardingen

Port Sunlight

Interdependent

Shanghai

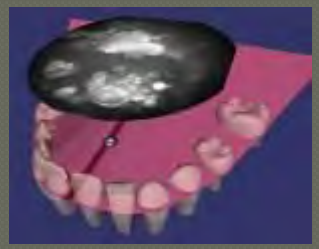
Trumbull

Bangalore

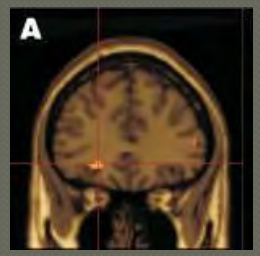
Science Expertise, Key Facts & Figures

Structured Materials and Process Science

Bioscience



Advanced Measurement and Data Modelling



Sensation, Perception and Behaviour

Nutrition and Health

- Total of 6000+ R&D professionals
- 6 Global Research Centres
- Unilever holds 20,000 granted and filed patents worldwide

About this Talk

- This really evolved from my own experiences of using COMSOL, which I started about 2-3 years ago.

- This incursion was more from need when I realized that it was not possible for me to conduct a particular experiment, and I needed some predictive capabilities for a problem that I was working on.

- I spent half a day on COMSOL and got this done (it was a simple problem, and I kind of knew the physical interpretation and the expected solution). I, of course, discussed this with my colleagues, Theorists, and apart from verifying the correctness of the solution, realized the differences in approaches to a problem between us (experimentalists and theorists) and the use of terminology/instrumentation in both classes that either of us had a problem in taking up. This sat me thinking on the current topic, and thanks to the Invitation from COMSOL, has helped me research this difference and crystallize my thoughts into this talk.

- *Disclaimer: In preparing this, I have relied heavily for information on the Wikipedia and the references there in. While the information is sourced from there, I can claim my contribution to be the thought behind this and the inter-linkages that I hope I can capture and share with you today.*

Outline

- The earliest experiment
- History of experimentation
- Do we have a larger faith on experiments?
- Is Hypothesis *aka* "Theory", to be followed by a "experiment"?
- "Thought Experiments", origin of Simulation?
- Simulations: An alternate "Experiment"
- Conclusion

The Origin of Science/Thought

- The history of science is as old as the origin of life. With Curiosity, began science.
  - "Three apples that changed the world: Adam and Eve's apple, Newton's apple and finally, Steve Jobs's Apple" *Twitter comment on Steve Jobs's demise.*

Plato (428-348 BC)

- However, in recorded history
  - Discovery of Fire- 300,000 to 400,000 years ago
  - The beginning of Philosophy with Plato (428-348 BC) and Aristotle (384-322 BC)

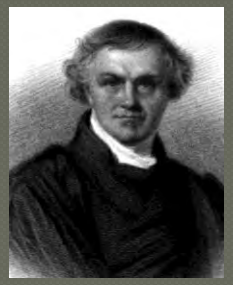
Aristotle (384-322 BC)

The Organization of Thought

- Philosophy was the forerunner of Science, and began with the organization and recording of the thought of early thinkers and philosophers, where observation and experience came together.
- The earliest paradigm of structure was in 'Empiricism' (from Latin experientia) in the philosophy of science, which emphasizes evidence, as comes from experience.
- History of scientific methods
  - rationalism, advocated by René Descartes (1596-1650);
    - "any view appealing to reason as a source of knowledge or justification" (Lacey, A.R. ,1996, *A Dictionary of Philosophy*)''.
  - inductivism, with Isaac Newton (1642-1727) and his followers;
    - ''general statements based on empirical observations, which are subsequently generalized into statements which can either be regarded as true or probably true.''
  - hypothetico-deductivism, which came to the fore in the early 19th century, named so by William Whewell.
    - ''proceeds by formulating a hypothesis in a form that could conceivably be falsified/corroborated by a test on observable data.''


Rene Descartes


Isaac Newton


William Whewell

Experiments that changed the world

- The testing of the Hypothesis was the crux of the evolution of science, and the 'Testing' involved experimentation.
- Some of the Key insights into Life and the Physical World were established through experiments.
  - 1609 – Galileo Galilei observes moons of Jupiter in support of heliocentric model
  - 1665 – Robert Hooke, using a microscope, observes cells
  - 1796 – Edward Jenner: tests the first vaccine
  - 1801 – Thomas Young: double-slit experiment showing wave-particle duality
  - 1820 – Hans Christian Ørsted discovers the connection E&M
  - 1843 – Joule measures the equivalence of mechanical work and heat
  - 1859 – Charles Darwin publishes The Origin of Species (natural selection)
  - 1861 – Louis Pasteur disproves the theory of spontaneous generation
  - 1887 –Michelson-Morley experiment, showing that the speed of light is invariant
  - 1911 – Rutherford's gold foil experiment determines the shape of the atom

Was this the beginning for a Bias for experimentation?
Is experimentation more intuitive?

Evolution of 'Thought Experiments'

- Gedankenexperiment (literally thought experiment) was first used by Ørsted in ~1812.
- All thought experiments, employ a methodology that is a priori, rather than empirical, in that they do not proceed by observation or physical experiment.
- Thought experiment, "was the most ancient pattern of mathematical proof", where the emphasis was on the conceptual, rather than on the experimental.

Is this when 'Theory' began?

'Scientific' Theory

- "A theory is a good theory if it satisfies two requirements: It must accurately describe a large class of observations on the basis of a model that contains only a few arbitrary elements, and it must make definite predictions about the results of future observations." Stephen Hawking in A Brief History of Time
- Einstein's Special Theory of Relativity.
  - two phenomena that had been observed (his assumptions)
    - "addition of velocities" is valid (classical physics, relativity),
    - light did not appear to have an "addition of velocities" (Michelson-Morley experiment).
  - the speed of light is a constant (his prediction)
- A model is a representation to describe a manifestation of a phenomenon or the interaction among a set of phenomena. The phenomena themselves are governed by the laws of physics.

The Purpose of a Theory and a Model is prediction.

Is Theory then any different from experiments?

- There is an equivalence in thought between experiments and theory, though the methods are different.
- Experimentation did precede theorizing in History, probably due to the intuitive nature of experiments.
  - A child learns more by experimentation and getting it right! Could this have also been the natural evolution of humans?
  - The Conceptual framework for theorizing came with the rise of philosophers and thinkers and post the evolution of structured thought.
  - The tools for 'Modern Scientific Theory' evolved much later in history

If the Purpose of a Theory and a Model is prediction,
What were the *key enablers that catalyzed* this?

Key Enablers *for the growth of* Modeling & Simulations

- The power of predictions through modeling and Simulation, as we know today, was unleashed by the development of two key disciplines
  - Numerical Methods in Mathematics
  - Computing Tools and Techniques
- The two areas developed independently, with Computing following the developments in Mathematics by at least a century

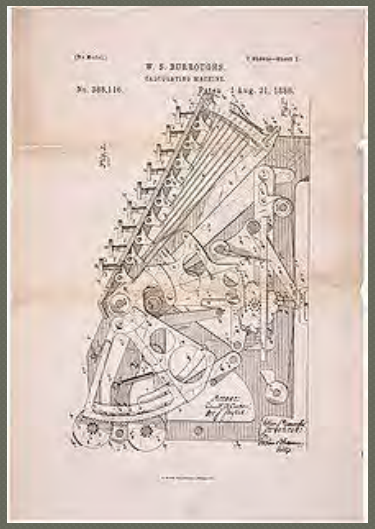
Evolution of Numerical Methods

- Numerical analysis is the study of algorithms that use numerical approximation for the problems of mathematical analysis.
- Obtaining approximate solutions while maintaining reasonable bounds on errors.
- Had nothing to do with computing, but began as early as BC 7289
  - Babylonian tablet gives a sexagesimal numerical approximation of ROOT 2.
  - Linear interpolation was already in use more than 2000 years ago. Many great mathematicians of the past were preoccupied by numerical analysis.
  - Names of important algorithms like Newton's method (written in 1669, published in 1711), Lagrange interpolation polynomial (1795), Gaussian elimination (1777-1855), or Euler's method (1707-1783).

Tools for Computations

- The earliest tool for computation was probably the abacus. …2400 BC
- Came out of the need for performing arithmetic processes

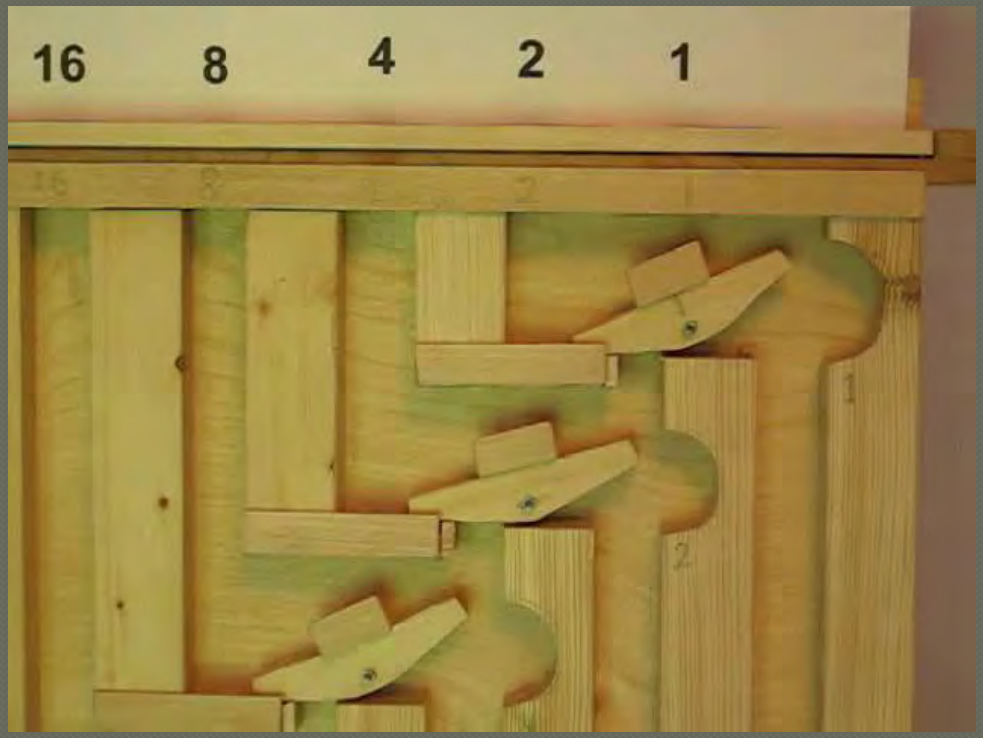
Slide Rule, 17th Century



Patent drawing for Burroughs's calculating machine, 1888.

Comptometer, Model ST (1930s)

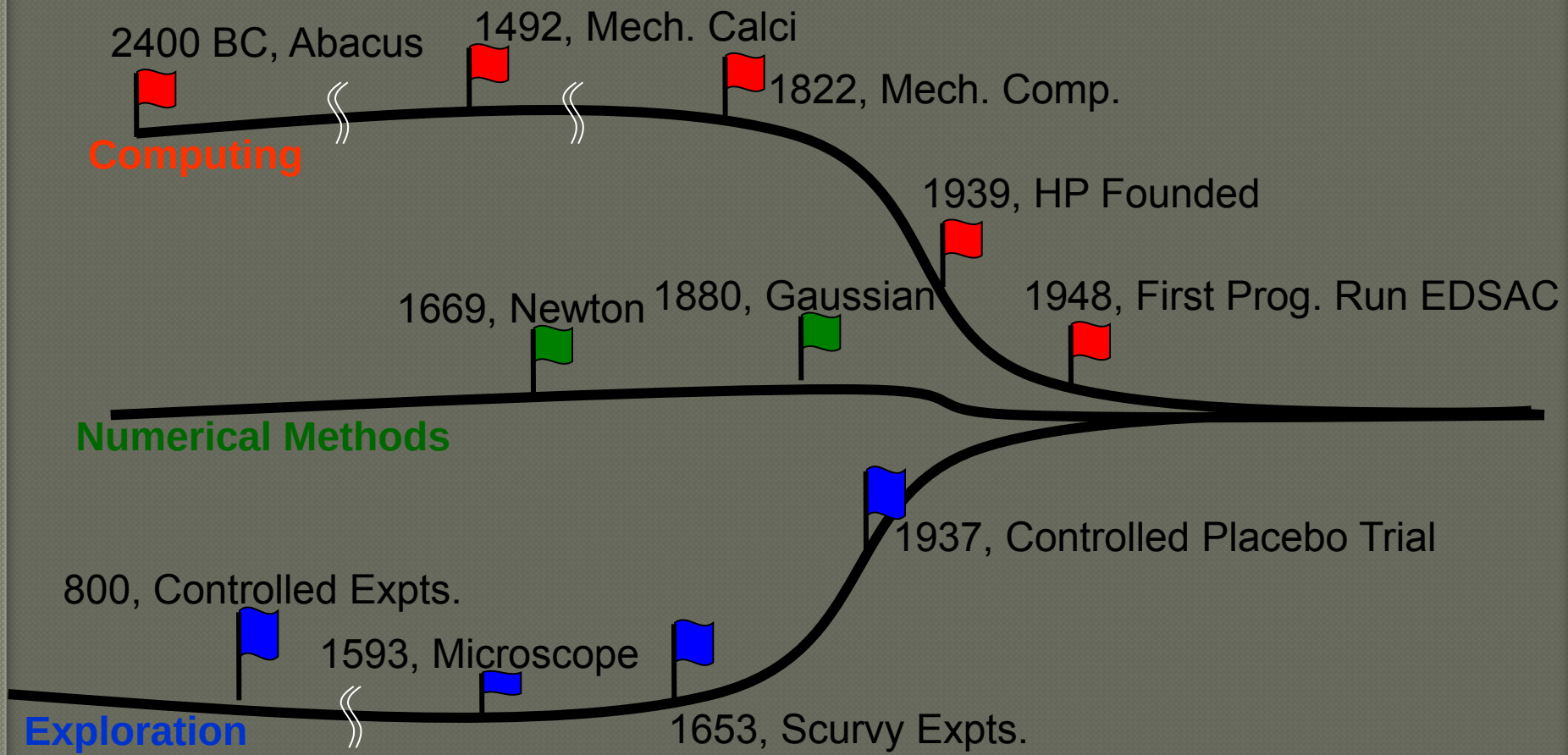
First all-electronic desktop calculator, Sumlock Comptometer Ltd, UK , 1961



http://www.youtube.com/watch?v=GcDshWmhF4A

http://woodgears.ca/marbleadd/ Matthias Wandel

Timeline for the development



The history of Computing and Simulations is less than 100 years old!

My Thoughts..

- Experiments are
  - "trial Solution to a Hypothesis!"
- Need tools/workshop for these trials (and skill)
  - 'Workshops' with
    - beakers and instruments
    - Computers and software
  - Different skills needed to work in these workshops, but a common Expertise
  - In spite of the expertise, the differing skills put an impediment in working in both of these workshops

Open Questions

- Has our education further biased us to experimentation?
  - Science practicals..Observation evokes interest.
  - Computer Sc. in school is about MS Word and PPt.
- Is abstraction harder to grasp?
  - Or are we just unable to share the excitement of science through 'virtual simulations'
- Are Students biased by this?

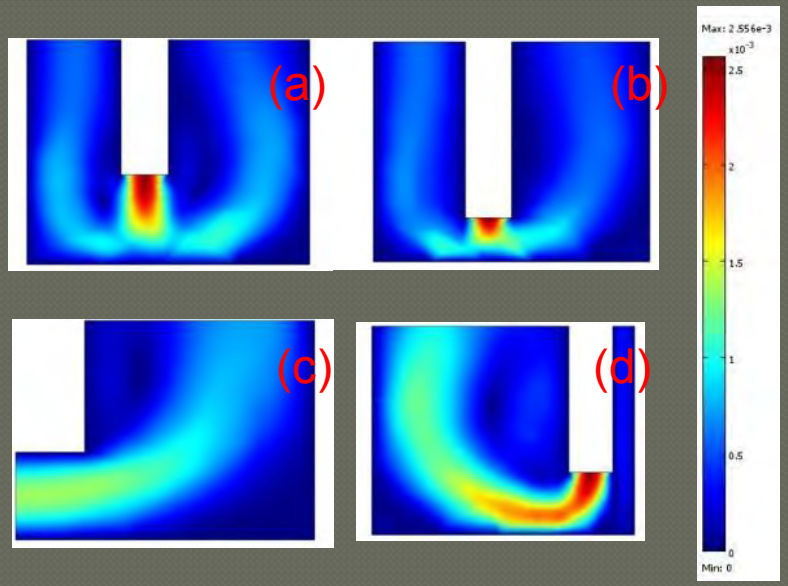
Is there hope for Experimentation through Simulation Tools?

- Ansys/COMSOL (MATLAB/CAD et al)
  - Allows for the interpretation of response of a cause in a Physical form, but in abstract space.
  - As valid an 'experiment' with data and interpretation
  - Sometimes easier and less expensive to set up.
- Two examples to make my case… and justify my presence here!

Modern Simulation tools have broken the barrier!

Example 1: Optimization of residence time

- Problem statement:
- Design of entry and exit positions in a flow chamber to provide a requisite residence time with minimal distribution, for a given input velocity.

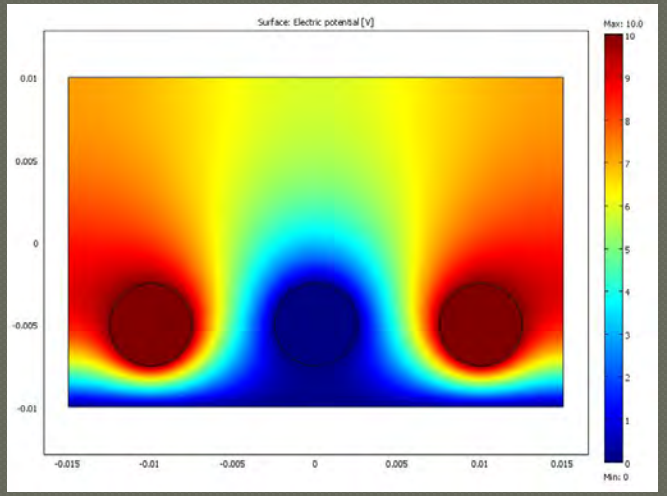


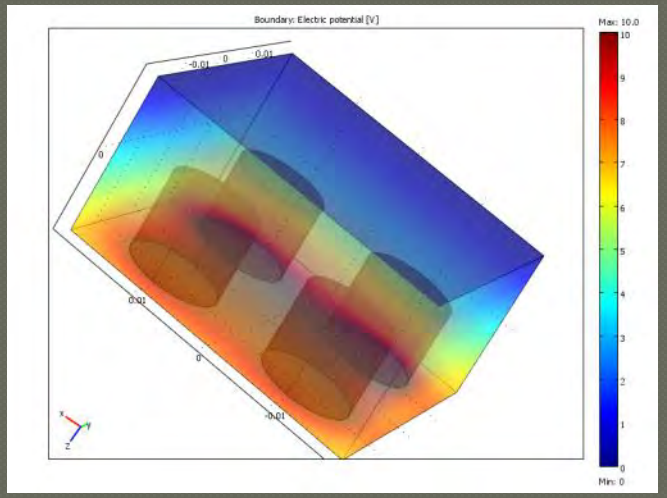
	Inlet (cm)	Exit (cm)	Residence time (s)		%
			Avg.	Min.	
a	2	10	308.5	186	60.3
b	2	10	299	156	52.2
c	4	10	297	132	44.4
d	2	10	306	156	51

Courtesy: Lalit Kumar and Jaideep Chatterjee

Example 2: Electric potential in an Electrolyte

- Problem statement:
- Predict Potential and electric field in a cell containing electrolyte for a given electrode configuration and potential.
- My Take:
  - Simple setup of the problem





A simplified model to predict the current–voltage relationship of an electro-chlorination cell; A Mukherjee, J Raut and R Venkataraghavan, J. App.Echem.: Volume 40, **9** (2010), 1659.

Conclusions

- The evolution of Science began with the beginning of curiosity.
- 'Experiments' led early philosophy, science
- The coming together of Mathematics, Computing (hardware and software) and exploration in early 20th century advanced theoretical studies. Simulations being the most impactful return.
- Comsol and others have played in crucial role in bringing both the experimentalist and theorist to a common plane…because exploration cannot be about one or the other.

Thank You

Acknowledgements

COMSOL
Colleagues
Unilever

Abstract

Science has progressed since the days of structured thought (~400 BC) to where it is today (when even a scientist is at sea when asked about a discipline that borders his). The pursuit of science has evolved from being a experiential reasoning with no boundaries to a highly complex, involved and technologically advanced area of study. Apart from being compartmentalized into disciplines of study, even the tools used are subject to the same compartmentalization. As a student having chosen to pursue science, an early decision of being a ''theorist'' or ''experimentalist'' needs to be taken, before you take the plunge. Has this changed in the last 15 years? Are simulation tools breaking the barriers for this? I think out aloud, as an experimentalist, if my dabbling with simulation tools has awakened hope that this 'barrier' can be broken. The talk will explore the epistemology of science, the history and evolution of science, and the interest in abstraction, origin of mathematical models and the growth of computer simulation more recently.

R Venkataraghavan,
for the Invited Keynote address at the Comsol Conference, Bangalore