

UNIVERSITY OF TWENTE.

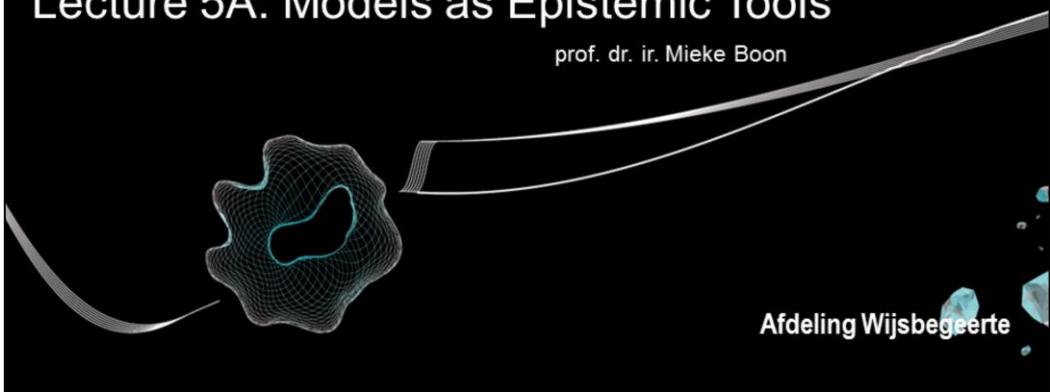


## Philosophy of Engineering: Science

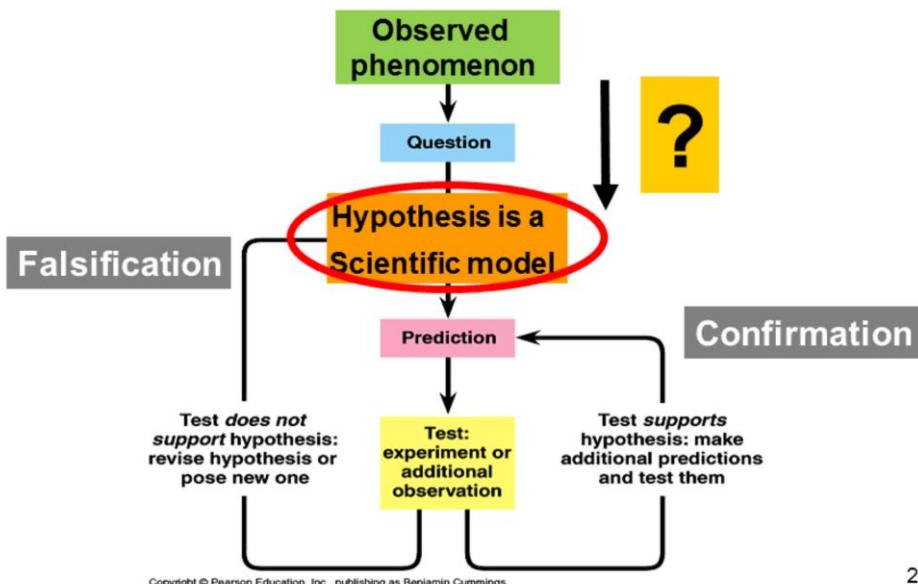
### Lecture 5A: Models as Epistemic Tools

prof. dr. ir. Mieke Boon

Afdeling Wijsbegeerte



# How do we construct a scientific model that explains the observed phenomenon?



Copyright © Pearson Education, Inc., publishing as Benjamin Cummings.

2

[See explanatory text in slides of week 4]

# How do we construct a scientific model that explains the observed phenomena?

**Criteria for evaluating the model:**

- Logical consistency
- Internal coherency
- Coherency with accepted theoretical knowledge
- Empirical adequacy
- Explanatory power
- Appropriateness to epistemic purpose(s)
- ...

**Ingredients (B&K):**

- Empirical knowledge & data
- Theoretical knowledge
- Scientific concepts

## Constructing a Model?

**Ways of Scientific reasoning:**

- Deductive reasoning
- Inductive reasoning
- Mathematization
- Idealization
- Explanatory reasoning (involves concepts, metaphysical picture, analogies, ...)/

**'Design' criteria for constructing the model (B&K):**

- Epistemic purpose of the model
- Measurement techniques
- Experimental equipment
- Mathematical techniques

## **The B&K Theory of Scientific Modelling:**

(Re-)construction of a model (e.g., as presented in scientific articles) involves asking: “What is ..”:

Note that the introduction of a scientific is usually much broader than the phenomenon at which the article will focus! => It is often hard to pin-point the phenomenon of focus, that is, the specific phenomenon investigated and modelled in the article. This is why this first step is very important and actually difficult:

- i. **Specific phenomenon (X) for which the ‘model of/for X’ is produced.**
- ii. ..

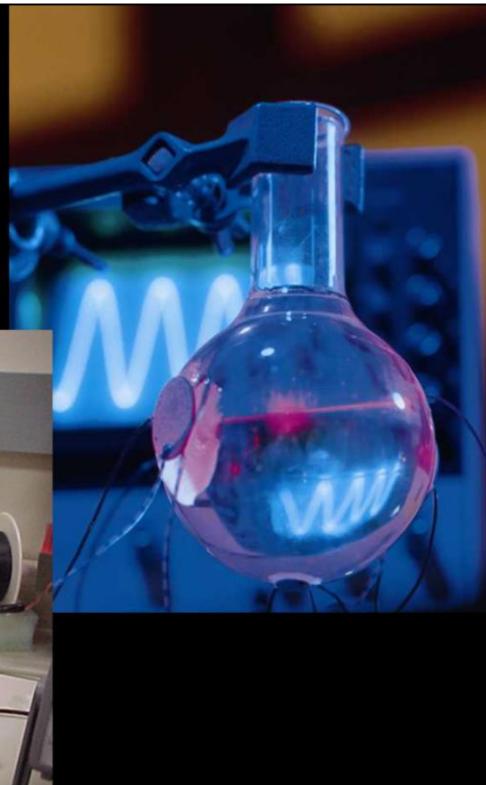
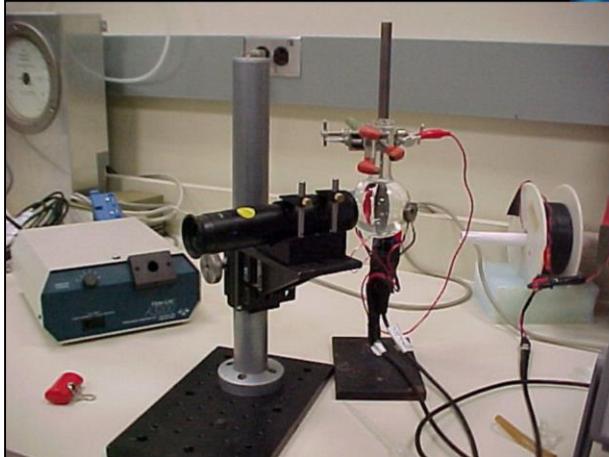
## **The B&K Theory of Scientific Modelling:**

(Re-)construction of a model (e.g., as presented in scientific articles) involves asking: “What is ..”:

- i. Specific phenomenon (X) for which the ‘model of/for X’ is produced.
- ii. Model type (e.g. morphological, logical, functional, mathematical, causal-mechanistic, statistical, ..).
- iii. ‘Epistemic purpose’ of the model.
- iv. Relevant (physical) circumstances and properties.
- v. Measurable (physical) variables.
- vi. Idealizations, simplifications, and abstractions.
- vii. Theoretical and empirical knowledge, and principles, used in the construction of the model.
- viii. Justification of the model.

# Explaining Sonoluminescence

Emission of a light pulse from imploding bubbles in a liquid when excited by sound.

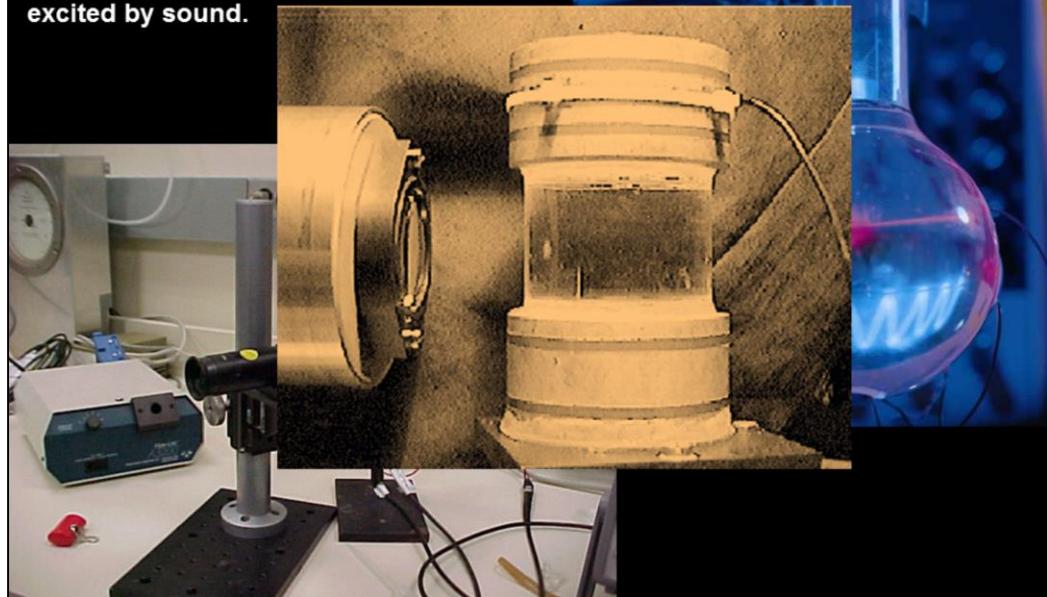


Apparatus for single bubble sonoluminescence. The ultrasound is applied across the rounded bottom flask and hence bubble is created.

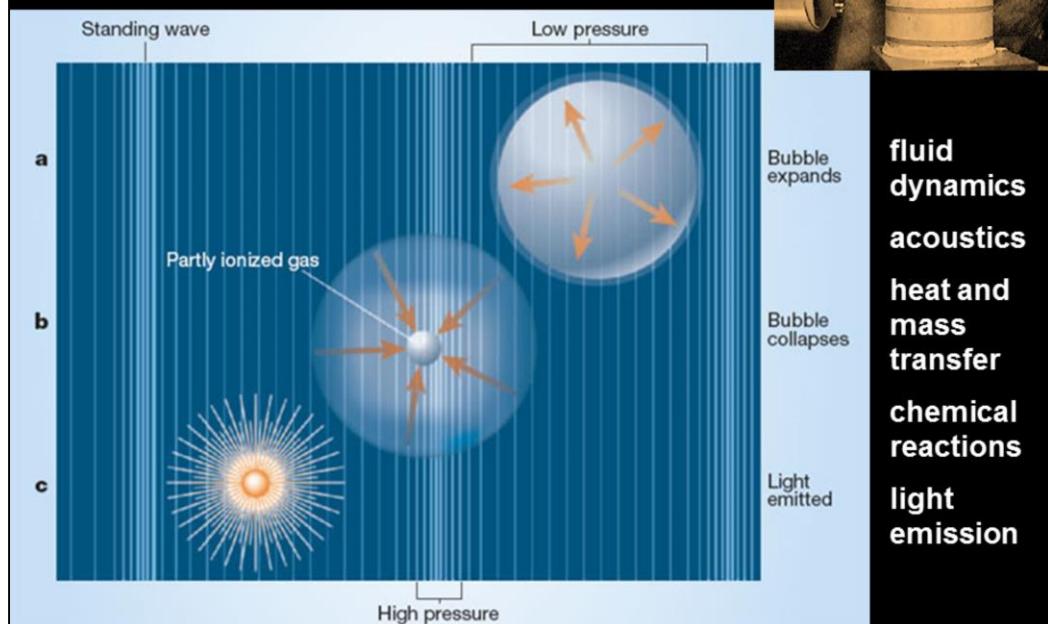
An example is how scientists developed an explanation of the phenomenon of sonoluminescence, which is the emission of a light pulse from imploding bubbles in a liquid when excited by sound. Brenner et.al. (2002, 427) state that "an enormous variety of physical processes is taking place inside this simple experiment [that produces the phenomenon of sonoluminescence], ranging from fluid dynamics, to acoustics, to heat and mass transfer, to chemical reactions, and finally to the light emission itself." What this example shows is that scientists are able to interpret a phenomenon (e.g. the emission of a light pulse from an imploding gas bubble), in terms of mutually interacting, physical processes for which accepted scientific explanations are available.

# Explaining Sonoluminescence

Emission of a light pulse from  
imploding bubbles in a liquid when  
excited by sound.



# Explaining Sonoluminescence: a causal + mathematical model



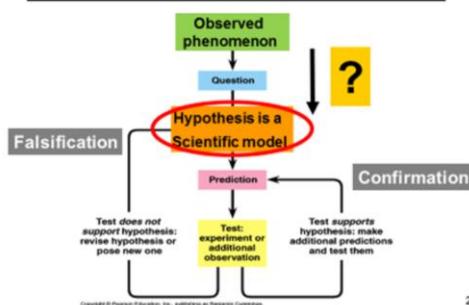
The construction of this model involves an interdisciplinary approach: many different fields seem to be relevant for understanding the behaviour of the bubble. Scientists know this based on knowledge of phenomena that occur at specific physical conditions. The causal-mechanistic + mathematical model was constructed by means of theories in those fields.

**Article “Single-bubble sonoluminescence” (see course materials for this scientific article by Brenner)**

- i. The phenomenon (X) for which the 'model for X' is produced? Light-flashes of bubbles in a standing sound-waves.
- ii. Model type? Causal-mechanistic as it presents the physical mechanism by which the phenomenon X is produced. But the authors also develop a mathematical model.
- iii. 'Epistemic purpose' of the model? Models are 'tools for thinking'. Causal-mechanistic models often are used for thinking about possible interventions (e.g., in the context of technological applications).
- iv. Relevant (physical) circumstances and properties? The kind of fluid and gas (composition of the gas); the frequency and energy of the sound-wave; the pressure and temperature of the liquid; bubble radius; etc. Usually, in our measurements, we can measure the properties and intervene in the physical circumstances.
- v. Measurable (physical) variables (usually related to former). Additionally we can measure: Intensity of the light-flash, spectrum and wave-lengths of the emitted light; etc.
- vi. Idealizations, simplifications, and abstractions. E.g.: "we have assumed that the liquid is isothermal and so have neglected the equation for the fluid temperature. As an approximation, the bubble's extension compared to that of the flask and that of the sound wave is neglected, as it is orders of magnitude smaller."
- vii. Theoretical and empirical knowledge, and principles, used in the construction of the model? (many theories are used – also see former slide -- e.g.) Classical theory of bubble dynamics; theory of cavitation collapse;
- viii. Justification of the model? E.g., comparison of measured variables and calculations.

Very short B&K analysis of the article by Brenner.

How do we construct a scientific model that explains the observed phenomenon?



2

## The B&K Theory of Scientific Modelling

- i. The phenomenon.
- ii. Model type.
- iii. 'Epistemic purpose'.
- iv. Relevant circumstances and properties.
- v. Measurable variables.
- vi. Idealizations.
- vii. Theoretical and empirical knowledge.
- viii. Justification.

The HD-method remains a general diagram of scientific methodology. The B&K tool helps us to understand how the hypothesis is crafted. As we have seen in the example of the scientific model that explains the observed phenomenon of sono-luminescence, the hypothesis (in this case, the scientific model) is constructed by putting together different aspects, which are pointed out in the B&K theory of scientific modelling. At the same time, we have also seen in this example, that 'sub-hypotheses' (e.g., of whether the temperature raises in a bubble when it is compressed by the sound wave) are tested 'in-between' during the process of modelling.



## Philosophy of Engineering: Science

### Lecture 5B: Methodologies in the Engineering Sciences

prof. dr. ir. Mieke Boon

Afdeling Wijsbegeerte

In society, there is a widely accepted belief that science does not give us truth. Some people even defend that everyone has his or her own truth. Such ideas have led to the loss of authority of science and scientific research. Some even think that there is a crisis of expert authority, or a crisis of scientific authority. At the same time, society depends on scientific research for dealing with societal issues and challenges. This seeming controversy (or at least, tension) is in need of an answer. More pressing, it is important to protect science against simplistic attacks. Examples of such attacks can be found in societal issues such as the climate debate (but also see for instance responses to this TED X lecture <http://www.tedxamsterdamwomen.nl/sprekers-2010/on-stage-trudy-dehue/>).

Furthermore, it is important that scientific practices improve as to meet serious difficulties and limitations of current approaches. Besides other things, the current societal situation and the practical/methodological challenges of scientific research imply that we are in need of more refined ideas about science and scientific research.

Academically trained professionals and researchers have the task to speak about science and to explain for themselves and for the general audience what science is and can do for us – but also why it is limited. Also, finding ways to improve scientific approaches in your own profession requires a

better understanding of science. One of the biggest challenges for scientific researchers and professionals today, is dealing with complexity and the fragmentation of knowledge. This involves, for instance, working interdisciplinary, multi-disciplinary and trans-disciplinary – which is difficult, and often not part of our academic training. In this course it is suggested that scientific researchers and professionals are better prepared to meet this challenge when having a better understanding of science at a kind of ‘meta-level’.

Philosophy of Science deals with these issues as it asks questions such as ‘What is science, and why/when is knowledge called scientific?’ ‘Whether or how scientific knowledge can be proven / justified?’ ‘What does it mean to say that knowledge is true?’ ‘Why should we rely on science?’ ‘How should we conceive of the relationship between knowledge – which is in the domain of language – and the real world?’

The first part of this course has focused on learning a vocabulary and ‘doing philosophical analysis’, by means of which some naive ideas about science and scientific knowledge have been made visible. These philosophical analyses aimed at doing two things. Firstly, making explicit the kind of (philosophical but naive) ideas about science and scientific knowledge that are held by many people. Secondly, to explain why/how such ideas, when analyzed in more depth, indeed support skeptical claims about science.

In the last few decades of the philosophy of science, this situation has led to the so-called ‘Science wars’ [http://en.wikipedia.org/wiki/Science\\_wars](http://en.wikipedia.org/wiki/Science_wars). Said rough and dirty, the one camp aimed to defend the authority of science by claiming that science is objective and can give us truth. This position is defended, for instance, by a tradition called ‘Scientific Realism’. The other camp defends that science is subjective (so, a mere social enterprise driven by blind ambition in which we aim to prove what suits us, etc.). The latter position is defended, for instance, by a tradition called ‘Social Constructivism’ (the slogan is that ‘scientific knowledge is a social construction’). [Part II of Ladyman, which is not part of the compulsory materials of this course, explains and discusses these positions].

In the last class, I have introduced the outlines of an alternative approach, which is at the frontline of developments in the philosophy of science. This new approach aims at an alternative understanding of science, aiming to do justice to previous philosophical insights, and aiming to ‘solve’ part of the controversies. This alternative understanding of science (or shortly, ‘picture of science’) aims to give you clues for thinking about scientific research in a new way as well.

This new approach goes back to the assumption central to the whole debate and to a widely accepted ‘picture of science’, namely that scientific knowledge (firstly) is a representation (picture or description) of ‘the world behind the perceivable phenomena’. Developing the alternative starts from a non-representational understanding of scientific knowledge. As an alternative, it is suggested to consider scientific knowledge firstly as ‘tool for thinking’ rather than a representation of ‘what the world behind the perceivable phenomena is like’. (for an explanation of the contrast between ‘scientific knowledge as a representation’ versus ‘scientific knowledge as epistemic tools’, see the notes that go with the last slides of Lecture 4). The idea is that scientific knowledge is not firstly meant to be a representation (a description or a picture). Instead, scientific knowledge is constructed in the context of certain epistemic uses. This idea agrees to how we usually deal with knowledge: we ask, ‘What can we do with it?’ ‘What are the consequence we can predict with it?’ This is what I mean by ‘epistemic use’. We use the knowledge to think and to come up with new ideas – knowledge such as represented in scientific models enable us to think creatively and critically and ask new questions. It enables us to perform thought experiments, think up real experiments and technological devices, to forecast new situations, make calculations, and to build computer simulations etc.

Note that in this alternative we abandon the idea that scientific knowledge is true, as the ‘truth’ of scientific knowledge means to say that the knowledge corresponds to, or correctly represents the real world.

Giving up on the truth of scientific knowledge may suggest that ‘anything goes’, and that scientific knowledge is very subjective or arbitrary. But this is a wrong conclusion. We still have some other very rigorous epistemic criteria for the acceptance or rejection of scientific knowledge. Firstly, scientific knowledge must be ‘empirically adequate’ (recall: empirical adequacy means that the perceivable – measurable, observable, etc. – facts predicted by the scientific knowledge under test should be true). In our method of testing a hypothesis (e.g. a scientific model) we still apply the HD method [see slide 3 of Lecture 4, which shows how the testing of a hypothesis involves both epistemic criteria ‘truth’ and ‘empirical adequacy’.] Furthermore, scientific knowledge (such as the knowledge represented in a scientific model) should be logically consistent internally, and it should be logically consistent and coherent with relevant, accepted theoretical knowledge and empirical facts. Other criteria important for the way in which scientific knowledge is constructed, are pragmatic criteria, which have to do with the practical usability of knowledge. Examples of pragmatic criteria are: simplicity and generality, but also specificity depending on the epistemic aim. Still another important criterion is ‘explanatory power’ – which is about the possibility of

drawing (new) cause and effect relations. We may, for instance, construct a very complicated algorithm that describes empirical findings very accurately (meaning that it is empirically adequate!), but its 'explanatory power' is limited in case this algorithm does not enable the researcher to draw meaningful relations between possible experimental interventions and consequences.

In brief, the construction of scientific knowledge has to meet a lot of epistemic and practical criteria. When briefly reflecting on these criteria, you may recognize indeed that they all have to do with the epistemic uses of scientific knowledge. Conversely, the epistemic usefulness of scientific knowledge is not an accidental by-product, but instead, it is intended to be that way – in other words, scientific knowledge is intended to be an epistemic tool. So, 'logical consistency' (and also mathematical consistency) of a theory warrants that we can reason with it anyway. 'Empirical adequacy' of a theory warrants that we can use it for making correct predictions (although we do not have certainty that every new prediction is correct!). Coherence with accepted empirical the theoretical knowledge adds to the empirical adequacy of a theory, and links it to other bodies of knowledge (providing the formation of networks between knowledge by means of which we can reason from one end to the other). Simplicity warrants that humans/scientists can employ scientific knowledge (laws, models, theories) in their scientific reasoning. These examples shows that knowledge is constructed such that we can use it in scientific reasoning about the world.

At this point, you may recognize that in this alternative picture of science, focus has turned from the relationship between 'scientific knowledge' and 'real world', to: '**how scientific researchers and professional engineers reason and think**'. Note that the Camera Obscura metaphor of knowledge (see slides Lecture 4) warranted the objectivity of knowledge because the real object is passively projected on the screen. Humans do not play any role in how this picture of the candle (= scientific knowledge) comes about. In the proposed alternative, the construction of 'scientific knowledge as an epistemic tool' is entangled with (or, 'matches to') the ways in which humans think and reason!

The idea is that scientific knowledge about a phenomenon of interest (e.g., a property, a process, structure, etc., which may be physical, but also mathematical; and in the social sciences, 'sociological') is constructed for epistemic purposes, i.e., for epistemic uses by humans – for instance, to create or change or optimize a property or process.

A consequence of the idea that scientific knowledge of a phenomenon is constructed for epistemic purposes is that we may ask how it is constructed –

is there some kind of common structure in how scientific researchers (now and in the past) construct scientific knowledge? The claim (made in the last lecture) is that there is indeed a common structure, namely, a collection of aspects that usually play a role in the construction of a model. This 'explanation' of how scientific models are constructed, is called the **B&K theory of scientific modeling**. The list of aspects can be found on the slide below.

Conversely, when trying to understand scientific knowledge (in particular, a scientific model), the easiest way to 'roughly understand' the scientific model is by analyzing the scientific article or the report of a scientific research project in terms of these aspects – in short, by actively searching for these aspects. The examples below illustrate very briefly how this works in analyzing a scientific article on the scientific model of the phenomenon called 'sonoluminescence'). The final assignment aims to exercise this approach [READ HANDOUT B&K Theory].

## What is Engineering Science?

---



How would you define 'engineering science' /  
What is 'engineering science'?



The topic of the class of today is methodologies in the engineering sciences.

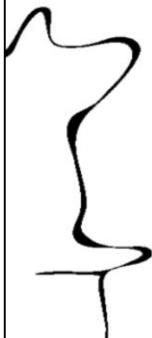
In reflecting on the questions (on this slide), you mainly focused on the differences between other natural sciences and 'engineering sciences.' You believe that knowledge produced in the engineering science is more practical, less general, less explanatory, less 'fundamental' and less 'deep', and that engineering sciences is problem oriented (or, oriented at solving problems). Also, the aim of other sciences is knowledge or theories, whereas the aim of the engineering sciences is technology and application.

What you say is partly correct. At the same time, it is important to recognize the similarities between scientific approaches of 'other natural sciences' and the engineering sciences. Furthermore, your view of 'real science' as opposed to 'engineering sciences' may be too idealistic, thus thinking with too much admiration of 'real science', and with too little appreciation of the engineering sciences. This is important, because in the pecking order of science, the engineering sciences often stand low in the hierarchy, which is unjustified. Certainly, there is low level engineering science, but this also is true about 'real science'. Furthermore, big discoveries usually result from many tiny little steps in scientific research. So, also when you would look at 'real science' you usually won't witness big discoveries.

In this course, I suggest that there are indeed significant differences between the engineering sciences and other natural sciences, but that the methodologies such as outlined in the HD method and B&K theory do apply to much of the scientific research in the engineering sciences as well.

The class of today will present a rough definition and description of the engineering sciences, which aims at showing how it differs from other sciences. Next, an example from the engineering science will be introduced, and how the construction of this scientific model (the model of the ideal heat engine) can be analyzed by means of the B&K theory. This analysis also aims to **illustrate how researchers in the engineering sciences think and reason.**

## What is Engineering Science?



**How would you define 'engineering science' / What is 'engineering science'? (Selection of students' answers):**

1. Science focused on technical applications
2. The finding of new technologies for all kinds of purposes.
3. The science of how to solve technical things.
4. It is a program that emphasizes enhanced understanding and integrated application of engineering, scientific, physics and mathematical principles.

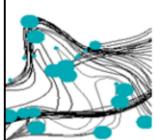
The most relevant difference between engineering sciences and other sciences is that it is scientific research performed in the context of a technological application. Putting it this way is more precise than saying that engineering sciences aim at applications (which is not wrong, but only roughly correct), as the production of knowledge, of scientific models, of scientific understanding, of scientific concepts, etc. is crucial to the engineering sciences – and which justifies that we call it *engineering science* rather than just engineering.

You may notice that the idea of 'scientific knowledge as epistemic tool' is more 'natural' for the engineering sciences than for (our 'traditional' understanding of) 'real' science': **In the engineering sciences researchers construct scientific knowledge such that it enables them to think of solutions and new technological possibilities!**

Here, I will briefly explain how the idea that engineering science is 'scientific research in the context of technological applications' points at some differences between the engineering sciences and other natural sciences.

This definition entails that the physical phenomena (properties or processes, etc.) for which researchers in the engineering sciences produce scientific knowledge usually are technologically generated. In other words,

technological devices produce phenomena that are, or may be of technological interest. Put still differently, the engineering sciences study technologically produced 'physical' phenomena. [In electrical engineering, think of electrical signals that are technologically produced and controlled].



## What is Engineering Science?



**How would you define 'eng sc' Students answered:**

5. A branch of knowledge that looks for an explanation for the different phenomena in nature. This explanation is made through modeling describing how stuff work or behave.
6. For me engineering science means applying engineering methods (like modelling) based on scientific knowledge.
7. Using fundamental sciences (laws of nature) and mathematical modeling to explain certain phenomena in nature and apply these phenomena to create products.

Apparently, this is different from 'real science', which studies 'natural phenomena', and maybe even, the basic 'building-blocks' of nature. This seems to point at a fundamental difference between the engineering sciences and 'real science': 'real science' studies 'Nature' whereas the engineering sciences study technology. However, when looking more closely at real research practices, most of the phenomena studied in 'real science' also have been produced by means of technological instruments. [An issue I will not discuss here, is whether the naive idea on the relation between the studied phenomenon and the technological instrument is always correct, namely, that a phenomenon is somehow 'put in the instrument', and just made visible by means of the instruments, rather than being 'produced' by it.] The engineering sciences and other natural sciences, actually, are very much similar in studying phenomena that are technologically generated.

Yet, a characteristic of the engineering sciences is its focus on how technological devices produce a phenomenon, and/or how to technologically intervene with a phenomenon (e.g., in order to improve or control it). As was said, other sciences do use technological instruments as well, but in the general picture of 'real science' these instruments often are kept out of sight. Think for instance of how scientific knowledge is presented in your physics textbooks (e.g., the Bohr model of the hydrogen atom, used as an example in this course). Textbooks often ignore the instruments, experimental model systems and experimental procedures by means of which the observable

phenomenon was produced for which the scientific model was constructed (e.g., the spectrophotometer etc.). When taking a look at scientific articles, however, it will often be difficult to make a clear distinction between the approach and content of articles produced in real sciences and the engineering sciences: their scientific approach is very similar. Nevertheless, articles in the engineering sciences emphasize the technological application context of the reported research (in the introduction of the article) and the applicability of the results (in discussion and conclusion section).

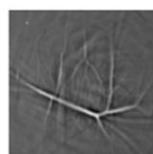
Furthermore, because the technological application context involves criteria such as feasibility, efficiency, specificity, reliability, etc., the engineering sciences put much more focus (mathematical) modeling variables related to these criteria (such as rate, error, selectivity, etc.)

The application context of the engineering sciences is technological instruments and the (innovative) technological application of technologically produced phenomena (properties and processes). The aim of other sciences is firstly, scientific knowledge or theories isolated from the technological devices involved. Although this distinction is too simplistic, there is a point in holding that the engineering sciences study phenomena that are of technological relevance, and also, that they study the technological instruments and procedures by means of which those phenomena are produced or manipulated. In other words, the engineering sciences do not only produce scientific models for phenomena, but also scientific knowledge (scientific models) of the workings of technological instruments and how these instruments produce the phenomenon of interest (including its quantification).

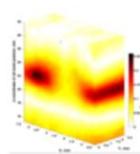
In brief, due to focus on technological application, the roles of technological instruments (how to make them, and understanding their effective and efficient workings) and technological procedures (e.g., for measuring, data processing, control, ...) is of direct interest to the engineering sciences. Scientific research for understanding phenomena (that are of technological interest) is very similar to scientific research in other sciences. Next to that, the engineering sciences also study how to make technological instruments – which goes hand-in-hand with aiming at understanding their workings – and how to perform technological procedures such as procedures for correct and efficient measurements, data processing, control, etc. Not only scientific knowledge of technological produced phenomena, but also scientific knowledge of technological instruments and procedures involved is relevant for the technological application.

One final remark may explain why the widely spread (but partly flawed) picture suggests a 'fundamental' difference between 'real science' and engineering science. See next slide.

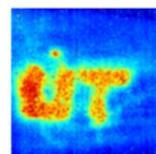
We investigate the use of light for medical purposes. Our final aim is to develop optical and hybrid optical-acoustical technologies for medical diagnosis, in particular in the fields of oncology and wound healing. Physiological properties of primary interest to us are microcirculatory blood flow, hemoglobin concentrations, and blood oxygenation. Our approaches include physical research into light-tissue interaction and its measurement, biomedical engineering to realize suitable instrumentation for *in vivo* use, and clinical evaluation together with several medical partners.



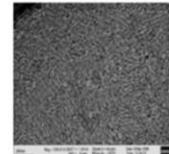
Photoacoustic imaging



Acousto-optic imaging



Flow measurement with dynamic optical speckles



Contrast enhancement of photoacoustics using gold nanoparticles

- <http://www.utwente.nl/tnw/bmpi/posters/>
- [http://www.utwente.nl/tnw/bmpi/posters/2013/Munich\\_Poster.pdf](http://www.utwente.nl/tnw/bmpi/posters/2013/Munich_Poster.pdf)
- <http://www.utwente.nl/tnw/bmpi/publications/>

This example illustrates how the widely spread (but partly flawed) picture, which suggests a 'fundamental' difference between 'real science' and engineering science, is kept alive by the scientific community itself.

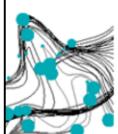
In selling their research to the 'outside' world, researchers in the engineering sciences usually focus on the technological (and societal) relevance of their research. They focus on the technological application context by explaining the technology and its advantages. Thereby they suggest that they work primarily on the development of a technology as engineers, which often is not the case. In public media, researchers hardly speak about the scientific research they do and the scientific articles they write. Even students often do not notice this discrepancy between what researchers talk about and what they actually do most of the time. This is not because researchers want to hide something, but because the general audience usually is more interested in practical results.

A striking example is how the work of the BMPI research group of professor Wiendelt Steenbergen is presented to the outside world. Steenbergen is famous for developing Pammography. He recently was nominated for an innovation price for this new technology (see <http://www.youtube.com/watch?v=XRTVrxJEiLM>). In this clip and other occasions, he tells how important and relevant this technology is (detection of

breast cancer through imaging with sound) and explains the advantages over the existing technology, Mammography, which is much more painful for women. Yet, most of the time researchers in this group are working on scientific topics such as explained on the website of the BMPI group <http://www.utwente.nl/tnw/bmipi/research/> showing what their scientific research and scientific articles are about. Here you can find out that, amongst other technologies, mammography is the application context of their research, but their actual scientific research firstly focuses on phenomena relevant for the (dis)functioning of these medical technologies – you can see this, for instance, when reading titles and abstracts of their publications <http://www.utwente.nl/tnw/bmipi/publications/>.

The point made here is not that this research group is doing something wrong – their way of communicating with the general audience is fully legitimate. Even, it is very important that scientific researchers aim to show the societal relevance of their work.

Yet, this example aims to explain how we (students and audience, policy makers, and also philosophers of science) easily get a flawed impression of the character of the engineering sciences and of how scientific research plays a role in the development of technology.



# Scientific research in the engineering sciences: An example from bioprocess technology



Research project in Engineering Sciences:

## Process optimization bioleaching processes (in mining industry)

1988-1996

Delft University of Technology

Department: Bioprocess technology

This research project takes place in a sub-field of chemical engineering => bioprocess technology => biohydrometallurgy. 'Hydrometallurgy' means chemical processes for the recovery of metals from ores by chemical conversions in water (which contrast with the use of high temperature processes such as roasting). 'Bio' means processes that make use of micro-organisms such as bacteria (which contrast with the usual use of chemicals in chemical processes). Micro-organisms usually need water to survive, so the hydro is kind of obvious. Note that hydrometallurgy is also a discipline, and interdisciplinary between chemical engineering and mining engineering.

In engineering sciences, scientific research often starts, or is related to a technological 'problem' or aim or design-task. The technological design context of this research project in biohydrometallurgy is: *Process optimization of bioleaching processes*.

What is bioleaching? Bioleaching as a technology for the recovery of metals (such as copper) from ores, is known as a [technology in the Roman iron age](#) already. But only in the 1950s, it was discovered that bacteria are somehow responsible for the dissolution of the metals from ore, and in the 1980s, parts of this technology are still archaic, using so-called [heap leaching technologies](#).

The research project discussed here started in 1987, and discovered in 1996 how bacteria dissolve metals from ore. Discussing this example of a research project aims to show how this discovery was made, and how this discovery has contributed to the optimization of the technology.

## 1980<sup>th</sup> Mining Industry: Heap leaching of Copper



17

At start of the project the following things were known.

Technology: heap-leaching – takes decades before a heap is empty.

(1950s) Bacteria such as *Thiobacillus-ferrooxidans* are responsible for dissolution of metals from ores.

Metals 'sit' in ores as oxides and sulfides.

These bacteria live at extreme conditions: low pH (between 1 and 2.5), and no organic 'food', usually at room temperature, but some strains are thermophiles living at temperature up to 90C.

In laboratory experiments, bacteria only dissolve metal-sulfides (such as chalcopyrite, CuFeS<sub>2</sub>; pyrite, FeS<sub>2</sub>; sphalerite, ZnS). A simple laboratory experiment consists of the following procedure: A weighed amount of pure metal sulfide and a weighed amount of medium (usually diluted sulfuric acid at pH 2, as this is their natural environment), kept and shaken at a constant temperature. Samples are taken at strict time-intervals, in which the concentration of metal-ions and iron-ions is measured, and the number of bacteria are counted. At the end of the experiment, the residual weight of solids is measured.

The same bacteria also oxidize ferrous iron (Fe<sup>2+</sup>) into ferric iron (Fe<sup>3+</sup>), and some of them but not all can oxidize 'reduced' Sulphur compounds such as Sulphur and S<sub>2</sub>O<sub>3</sub>.. In this oxidation they use oxygen (which is dissolved from

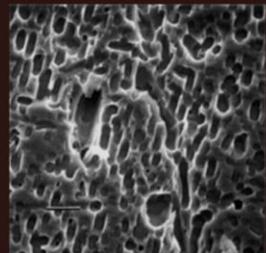
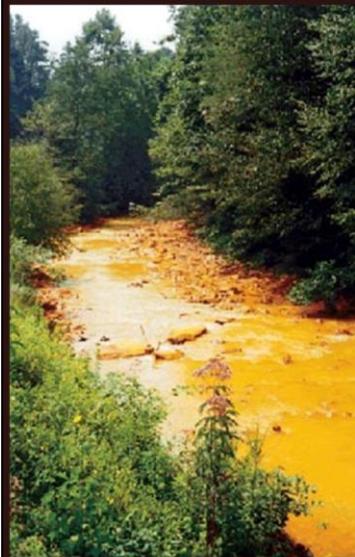
air into the liquid the bacteria live in).

These bacteria are called chemolithoautotrophs = use energy from inorganic compounds for their energy-uptake and carbon-dioxide for their growth, that is, producing organic matter. (CO<sub>2</sub> is dissolved from air into the liquid the bacteria live in).

## Mining Industry: Heap leaching of gold



## Phenomenon in nature: 'Bioleaching' = Bacteria dissolve metal sulphides ( $\text{FeS}_2$ )



## Phenomena observed in measurements and experiments

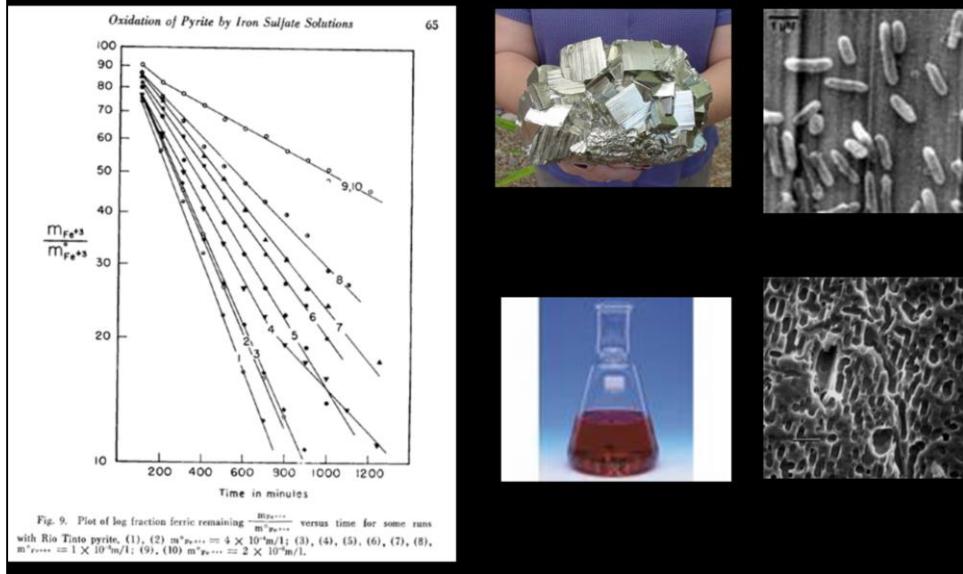
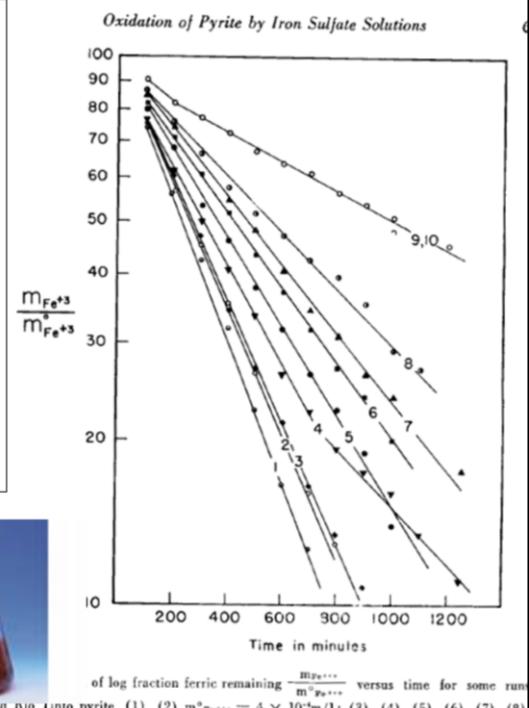


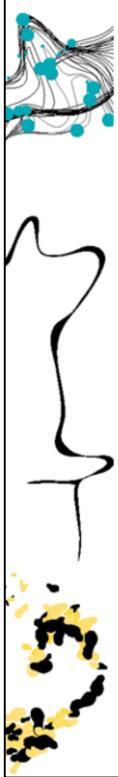
Figure 1. (a) Measured chemical pyrite oxidation rate in sulfate solution, normalized on the amount of pyrite. (b) Pyrite as a crystal. (c) Bacteria sitting on pyrite surface (Scanning Electron Microscope). (d) Shake flask with iron-sulfate solution as used in chemical and bioleaching experiments. (e) Pyrite surface after bioleaching: Holes apparently caused in the pyrite surface by the bacteria. (Scanning Electron Microscope).

## Relevant empirical knowledge: observed stoichiometry (equations)

direct	$\text{FeS}_2 + 15/4\text{O}_2 + 0.5\text{H}_2\text{O} \rightarrow \text{Fe}^{3+} + 2\text{SO}_4^{2-} + \text{H}^+$	bio	3a
incomplete	$\text{FeS}_2 + 2\text{Fe}^{3+} \rightarrow 3\text{Fe}^{2+} + 2\text{S}^0$	chem	3b
indirect	$3\text{Fe}^{2+} + 3/4\text{O}_2 \rightarrow 3\text{Fe}^{3+} + 3/2\text{H}_2\text{O}$	bio	4
	$2\text{S}^0 + 3\text{O}_2 + 2\text{H}_2\text{O} \rightarrow 2\text{H}_2\text{SO}_4$	bio	5
complete	$\text{FeS}_2 + 14\text{Fe}^{3+} + 8\text{H}_2\text{O} \rightarrow 15\text{Fe}^{2+} + 2\text{SO}_4^{2-} + 16\text{H}^+$	chem	3c
indirect	$15\text{Fe}^{2+} + 15/4\text{O}_2 + 15\text{H}^+ \rightarrow 15\text{Fe}^{3+} + 15/2\text{H}_2\text{O}$	bio	4

Measurements and experiments at different initial conditions. These authors conclude that those conditions are **relevant** since (as noting else changed) different rates are observed (the rate is represented by the slope of these lines => the process is faster at a steeper slope).



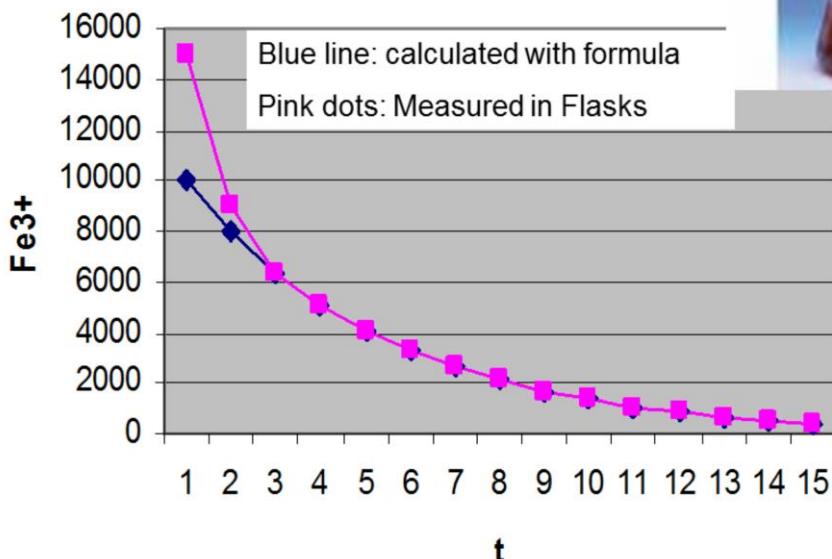


## What is engineering science?

### 1. Engineering science is scientific research in context of technological applications.

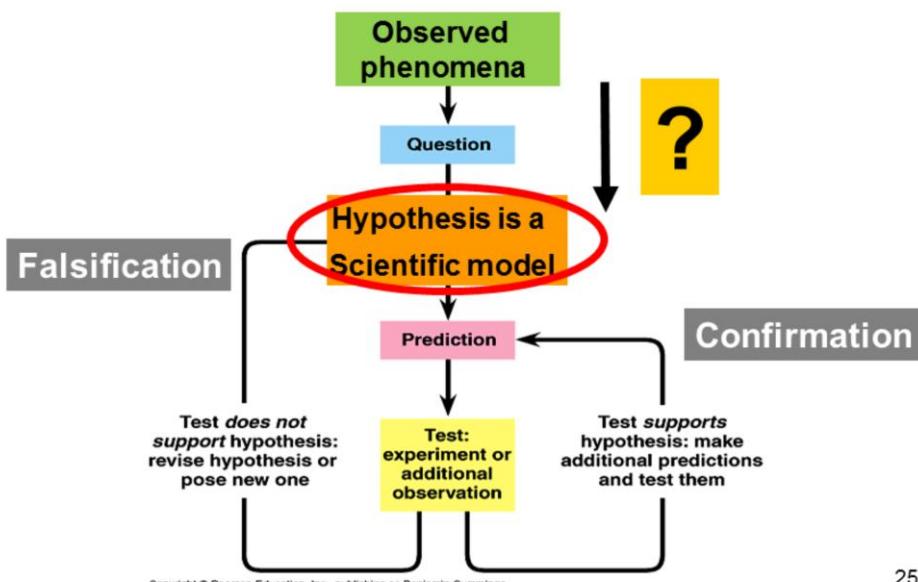
- ⇒ How is a technological problem (e.g., optimization of a process) translated into a scientific research project?
  - a. **Trial & error** approach (widely used in companies):  
Engineers fiddle with relevant variables to see whether it gets better.
  - b. Aiming at a '**more fundamental**' **scientific understanding** of the phenomena that determine the functioning of the technology (e.g., the industrial process of bioleaching) – (usually at universities).

$$\frac{d\text{Fe}^{3+}}{dt} = -k\text{Fe}^{3+}$$



Constructing a phenomenological law (law of nature?), which draws a relationship between measured variables.

# How do we construct a scientific model that explains the observed phenomenon?



Copyright © Pearson Education, Inc., publishing as Benjamin Cummings.

25

[See explanatory text in slides of week 4]

**Two competing mechanisms for explaining the dissolution of Pyrite by Bacteria such as *Thiobacillus Ferro-oxidans*:**



**Calculation:** assume a fully covered surface area with growing bacteria => small mathematical model can be generated => **Calculation** (using material specific parameters,  $Y_{sx}$  and  $\mu_{max}$ ), predicts that *direct* is far **too slow**

**Measurements** (at sterile conditions = measuring *chemical* oxidation rate of pyrite) show that *indirect* is far **too slow**



## What is engineering science?

---

### 1. Engineering science is scientific research in context of technological applications.

- a. Trial and error
- b. More fundamental' scientific understanding of the phenomena that determine the functioning of the technology ..
  - ⇒ Both hypotheses failed .
  - ⇒ Apparently, our scientific techniques are too limited
  - ⇒ **Scientific breakthroughs:**
    - By integrating different kinds of scientific modelling (e.g., theoretical-mathematical and causal modelling)
    - By developing new kinds of measurement methods and experimental techniques

#### 4.3.1 Batch and Continuous Cultures

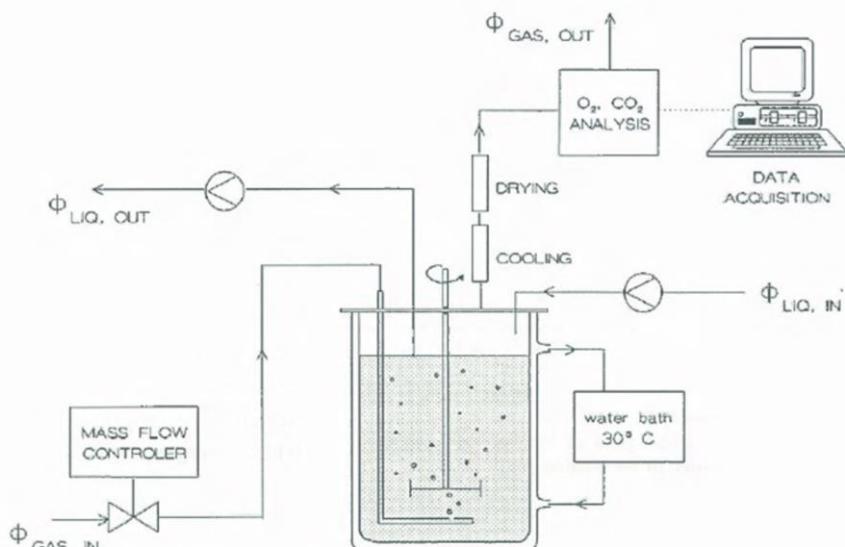
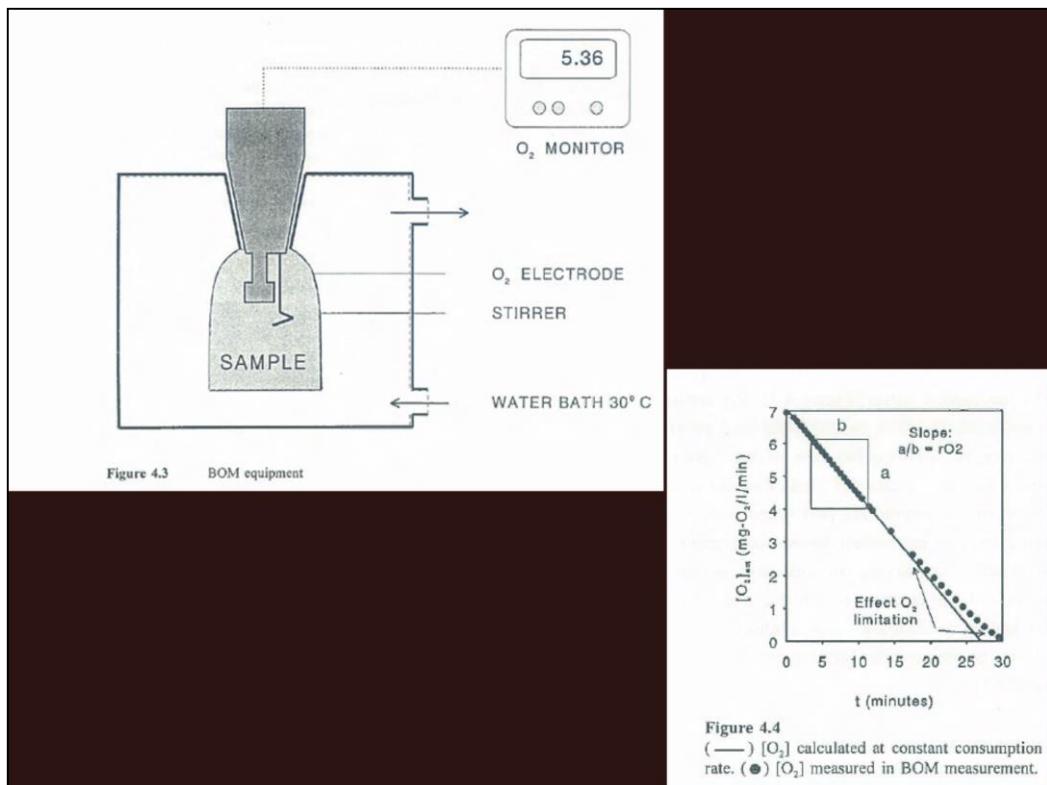
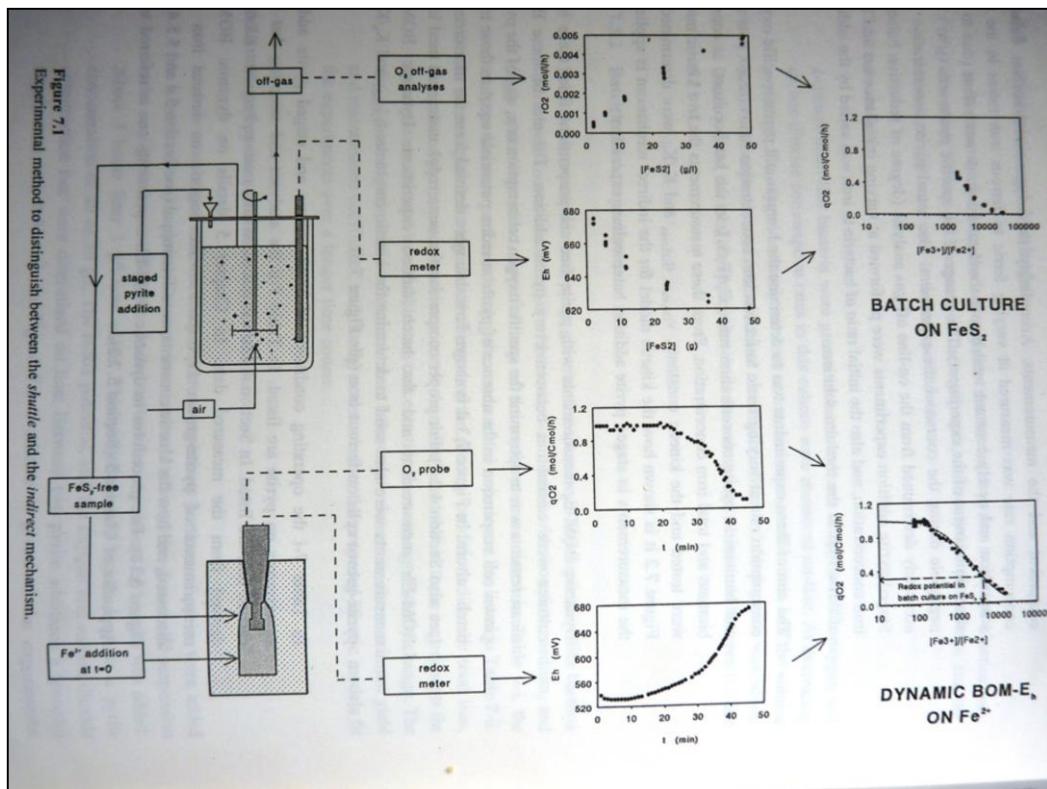


Figure 4.2 Fermenter equipment

Fermenter equipment. Commonly used in bioprocess technology, but new in bioleaching experiments (compared with shake-flasks). Crucial is the possibility of using of oxygen and carbon dioxide measurements in the gas that is used for aeration of the medium in which bacteria grow and oxidize the sulfide mineral. By means of mass-balances the (changes in) oxygen and carbon dioxide consumption in the vessel can be calculated.



A biological oxygen monitor (BOM) in which the dissolved oxygen concentration can be measured. This technique was combined with measuring the redox potential in a 'parallel sample' (see next Figure).



Measurement methods, and striving at consistency and coherency between data.

New experimental set-up in which the experimental techniques were combined.

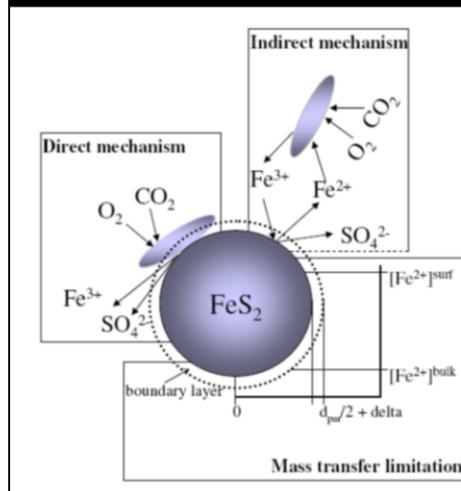


**The discovery of the scientific model  
(causal-mechanistic and mathematical)  
that explains how bacteria oxidize metal  
sulfides**

---

## Causal-mechanistic Model: How?

Indirect mechanism, but crucial is that chemical reaction rate is enormously accelerated by the value of the ferric over ferrous iron concentration ( $= [\text{Fe}^{3+}]/[\text{Fe}^{2+}]$ ), which is kept extremely high by the bacterial oxidation of  $\text{Fe}^{2+}$  to  $\text{Fe}^{3+}$ .



- 1 chemical pyrite oxidation rate:  $v_{\text{FeS}2} = -\frac{v_{\text{FeS}2,\text{max}}}{1 + \frac{1}{B} \frac{[\text{Fe}^{2+}]}{[\text{Fe}^{3+}]}}$
- 2 stoichiometry:  $v_{\text{Fe}^{2+}} = -15 \cdot v_{\text{FeS}2}$
- 3 stoichiometry:  $q_{\text{Fe}^{2+}} = \frac{q_{\text{O}_2}}{4}$
- 4 bacterial oxygen consumption rate:  $q_{\text{O}_2} = -\frac{q_{\text{O}_2,\text{max}}}{1 + \frac{K_S}{K_I} \frac{[\text{Fe}^{3+}]}{[\text{Fe}^{2+}]}}$
- 5 at equilibrium:  $[\text{FeS}_2] \cdot v_{\text{Fe}^{2+}} = C_x \cdot q_{\text{Fe}^{2+}}$

## Mathematical Model: How fast?

This set of mathematical equations describes the rates of the two phenomena involve: (1) chemical oxidation rate of pyrite,  $v_{\text{FeS}2}$ , which is accelerated by the ferric over ferrous iron concentration ( $= [\text{Fe}^{3+}]/[\text{Fe}^{2+}]$ ), and (4) the bacterial ferrous iron oxidation rate,  $q_{\text{Fe}^{2+}}$ , which is accelerated by a low value of  $[\text{Fe}^{3+}]/[\text{Fe}^{2+}]$ . This rate is measured by measuring the rate of oxygen consumption,  $q_{\text{O}_2}$ . The material specific parameters  $v_{\text{FeS}2,\text{max}}$ ,  $B$ ,  $q_{\text{O}_2,\text{max}}$ ,  $K_S$ ,  $K_I$  are considered (new) material properties, which can be determined in the experimental set-up that was developed.

The discovery. The explanation of bioleaching is an indirect mechanism: the sulfide mineral is oxidized by ferric iron ( $\text{Fe}^{3+}$ ) producing ferrous iron ( $\text{Fe}^{2+}$ ), which in turn is oxidized by the bacteria. The reason for the high bio-oxidation rate of the sulfide mineral is that bacteria maintain an extremely high redox-potential ( $\text{Fe}^{3+}/\text{Fe}^{2+}$  ratio), which speeds up the chemical oxidation rate.

Based on the experiments, next to this causal-mechanistic model, a mathematical model was constructed. This model entails the description of the chemical oxidation rate of pyrite ( $v_{\text{FeS}2}$ ) as a function of the ratio between  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$ , and the description of the rate at which bacteria oxidize ferrous iron ( $q_{\text{Fe}^{2+}}$ ) as a function of the ratio between  $\text{Fe}^{3+}$  and  $\text{Fe}^{2+}$ . Clearly, the rates work in opposite directions: Chemical reaction rate increases at increasing  $\text{Fe}^{3+}/\text{Fe}^{2+}$ , whereas the bacterial oxidation rate increases at increasing  $\text{Fe}^{2+}/\text{Fe}^{3+}$ . Equilibrium is achieved when the two rates become equal. These equations are directly coupled by mass- and stoichiometric balances.

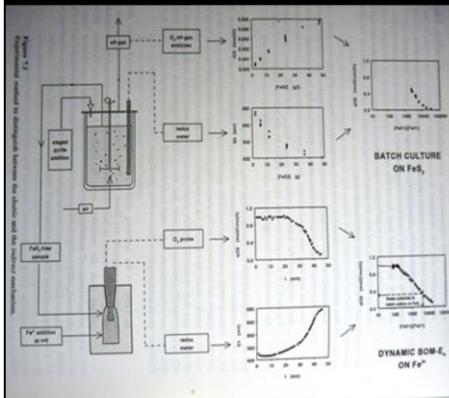
Note that the mathematical model involves four new parameters: two characteristic properties of pyrite -- namely, the maximum oxidation rate,  $v_{\text{FeS}2,\text{max}}$ , and a rate constant  $B$ ; and two characteristic properties of the bacteria – namely, the maximum consumption rate of the substrate,  $q_{\text{O}_2,\text{max}}$ , and a rate constant,  $K_S/K_I$ .

# Scientific explanation and mathematical modelling

Observation:  
Measurements

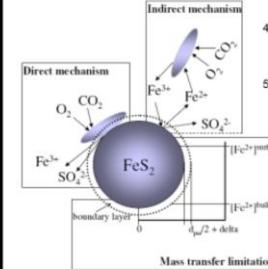
?

Hypothesis: Theory (or  
model)



Causal-mechanistic  
Model:

How?



1 chemical pyrite oxidation rate:

$$V_{FeS_2} = -\frac{V_{FeS_2,max}}{1 + \frac{1}{B} \frac{[Fe^{3+}]}{[Fe^{2+}]}}$$

2 stoichiometry:

$$V_{Fe^{2+}} = -15 V_{FeS_2}$$

3 stoichiometry:

$$q_{Fe^{2+}} = \frac{q_{O_2}}{4}$$

4 bacterial oxygen consumption rate:

$$q_{O_2} = -\frac{q_{O_2,max}}{1 + \frac{K_{O_2}}{K_f} \frac{[Fe^{3+}]}{[Fe^{2+}]}}$$

5 at equilibrium:

$$[FeS_2] V_{FeS_2} = C_f q_{Fe^{2+}}$$

Mathematical  
Model:

How fast?

Talking about 'scientific explanation' and 'having discovered the mechanism' is very suggestive towards a realist interpretation of the model: as if we have somehow observed that this is 'what the world behind the observable phenomena' is like, or, as if the scientist in a flash of inspiration saw before her mind's eye that this is what the world is like, and yes, this guess appears to be so successful that it must be true!

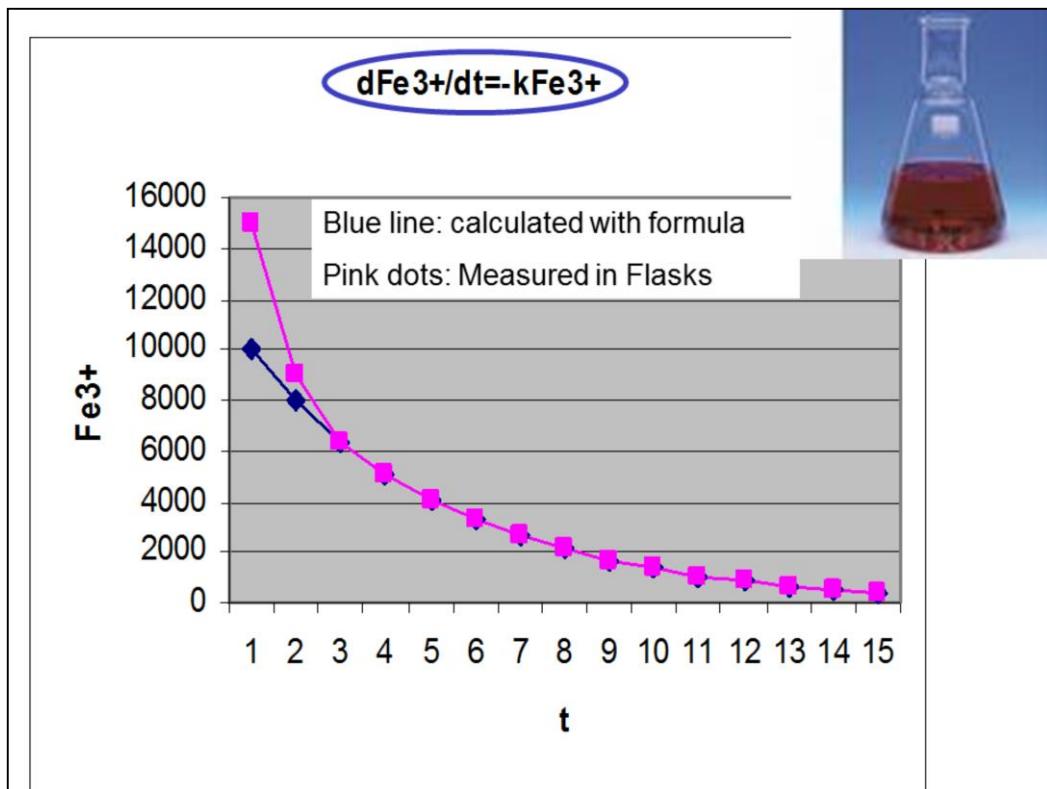
Is it possible to interpret this 'discovery' and the 'scientific explanation' from the anti-realist perspective?

In a realist view, we have a phenomenological world (observations and measurements), a real world (unobservable but causally responsible for the observed phenomena), and theories (or models) that are a kind of photographs or drawings depicting the real (but unobservable) world. So, on this picture, the semantic relationship is between the model and the real, but unobservable world.

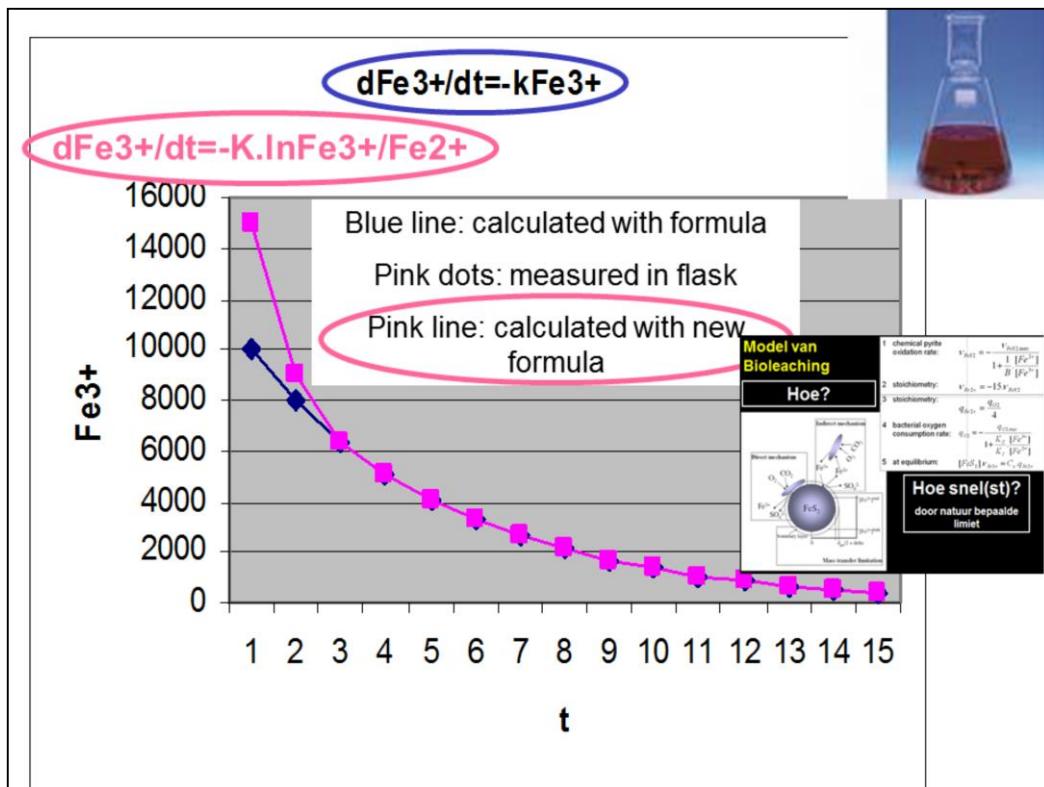
In the anti-realist alternative, it is proposed that the model (right hand side) is firstly related to observations and measurements (left hand side). On this view, scientists 'construct' coherent and intelligible models that enable them to reason about the system of interest. Importantly (and illustrated by this example), constructing relevant scientific models is dependent on the available ingredients: The more different kinds of measurements & the more

different kinds of experimental interventions with the system under study (producing new observable phenomena) & the more application of relevant theoretical and empirical knowledge, the more 'explanatory' the constructed model. "We cannot bake a good cake without such ingredients." On this view, the explanatory power is not related to some kind of magical vision of the world behind the observable phenomena, but rather, on the intricate relationships that are build between the ingredients mentioned.

The moral is that the model at the right-hand side would not have any meaning without the ingredients that play a role in their construction.



In the original articles that reported on chemical oxidation kinetics, authors claimed that the initial high oxidation rates were measurement errors. The newly discovered mechanism can explain these measurements. They are not errors.



Some remarks on what we can learn from this example:

[the graph is schematic; it does not show real data, nor their units.]

The blue equation in this graph is the original phenomenological description of the rate at which the mineral is dissolved, adopted by many authors at that time. The phenomenological description explains that the observed/measured metal oxidation rate is proportional to the  $\text{Fe}^{3+}$  concentration in the fluid. This phenomenological law (also called 'empirical law') is empirically adequate about the tail of the measurements ( $t=3$  onwards), but apparently not about the initial phase. The decision of researchers to discard of these 'outliers' at the start of the experiments makes sense, since in actual experiments, this phase only takes a few seconds, whereas the whole experiment takes days. Indeed, in the past, researchers considered these initial high values as outliers probably due to measurement errors, and accepted that the blue formula did not take these 'false data' into account.

The improved phenomenological description (the pink equation) also is empirically adequate. The new equation covers the initial 'outliers', and is an improvement as compared to the original blue equation, especially for describing the phenomenon (the oxidation rate) in those very first few seconds. The pink equation describes the mineral oxidation rate as proportional to the redox potential [which is a measure of the  $\text{Fe}^{3+}/\text{Fe}^{2+}$  ratio], instead of the original proportionality to  $\text{Fe}^{3+}$  only.

We learn from this example that phenomenological descriptions (the blue and the pink equation) build on what has been measured. These phenomenological equations aim at (a) describing patterns in the measured data, and (2) to make the equation as general as possible by introducing parameters,  $k$ , that are believed to be specific for a material or a system (e.g., the gas-constant, the elasticity constant, the electrical resistance of a material, etc). Note that this 'epistemic strategy' in scientific research is still very similar to what Boyle, Hooke, Ohm, Faraday and Balmer did in the past.

We also learn, therefore, that variables that are *not* measured do *not* occur in these phenomenological equations [it is not that the redox-potential as a measure for the ratio between  $\text{Fe}^{3+}/\text{Fe}^{2+}$  was not taken into account because scientists believed that it was irrelevant, but because they had not thought of using this measurement-technique]. The moral is that much of the developments in science are due to development, application and combination of new measurement techniques.

Another important thing to notice in this example is that, based on the new measurement-techniques in this research project (especially, the measurement of the redox-potential in the leaching fluid as a measure for the ratio between the concentrations of  $\text{Fe}^{3+}$  en  $\text{Fe}^{2+}$ ), scientists could come up with this improved *phenomenological description* of the process, yet, without any 'deeper' understanding of how bacteria dissolve the mineral sulphide (such as pyrite). In other words, in scientific research, we can choose to do different things: (1) we just search for phenomenological laws (= mathematical equations) that relate apparently relevant measured data in an efficient and empirically adequate manner, (2) or we try to come up with a scientific model that is explanatory richer of what happens in the process (as in the causal-mechanistic and mathematical model just shown).

Summarizing and applying some of the philosophical terms we have learned: although the pink formula is an empirically adequate 'law of nature', its explanatory power is very limited. Therefore, the improved phenomenological equation is poor as an epistemic tool for the original epistemic aim (the original epistemic aim was generating knowledge that helps in the optimization of bioleaching processes). Conversely, the model (the causal-mechanistic model, interrelated with the mathematical model that relates measured data) is a much richer epistemic tool for reasoning about possible improvements (optimization), or even new types of technology in bioleaching (= new design-concepts).

Indeed, it turned out that this improved understanding of the mechanism, together with the mathematical model that quantifies it, allowed for drafting

new design-concepts.

## Now: Bioleaching of Sulfide Minerals in Tanks



New design-concepts were based on the new understanding of the mechanism and mathematical model of bioleaching, which resulted in this type of industrial processes in mining industry. Instead of the traditional heap-leaching, currently, leach-tanks are used. Hence, process optimization indeed has been achieved by means of a scientific research project in which the observed phenomenon (bio-leaching) was explained and described by a causal-mechanistic and mathematical model. The original technology (heap-leaching) takes decades, whereas this process only takes a residence time (of the ore in the vessel) of one or two days.



## I. What is engineering science?

---

- 1. Engineering science is scientific research in context of technological applications.**
2. Engineering sciences strive to understand, predict or optimize the behavior of devices, and/or the properties of diverse materials, whether actual or possible.
3. The behavior or property is the phenomenon studied.
4. Engineering sciences aim at models for these phenomena (rather than at universal theories) – these models are presented in scientific literature.

## **The B&K Theory of Scientific Modelling:**

(Re-)construction of a model (e.g., as presented in scientific articles) involves asking: “What is ..”:

0. What is the technological problem to be solved?
  - i. Specific phenomenon (X) for which the ‘model of/for X’ is produced (**+ instruments producing it**).
  - ii. Model type (e.g. morphological, logical, functional, mathematical, causal-mechanistic, statistical, ..).
  - iii. ‘Epistemic purpose’ of the model.
  - iv. Relevant (physical) circumstances and properties.
  - v. Measurable variables (**+ instruments measuring it**).
  - vi. Idealizations, simplifications, and abstractions.
  - vii. Theoretical and empirical knowledge, and principles, used in the construction of the model.
  - viii. Justification of the model (**+ instruments in testing**).

In the engineering sciences, we usually start from a ‘problem-context’: a technological problem we wish to solve, or a technological function that we want to generate. Therefore, the very first question should be: *What is the technological problem to be solved?*

Often, a technological problem or a technological (dis)function is understood in terms of a (physical) phenomenon held responsible for the problem of (dis)function.



## **Final assignment (application B&K): How to read a scientific article in the engineering sciences?**

(see handout on B&K for  
instructions; and look at examples available in BB)

1. Choose a scientific article in which scientific modelling takes place.
2. Start with defining the technological context: Technological problem, technological function, phenomenon responsible for it that is examined and modelled.
3. Then apply step i-viii in order to understand the scientific work presented in this article.