

TNO report**TNO 2013 R10541****Enabling Technology Program Modelling
Midterm Report (2011-2012)****Earth, Environmental and Life
Sciences**Princetonlaan 6
3584 CB Utrecht
P.O. Box 80015
3508 TA Utrecht
The Netherlandswww.tno.nlT +31 88 866 42 56
F +31 88 866 44 75
infodesk@tno.nl

Date	15 April 2013
Author(s)	Dr. ir. E.W. Meijer Ir. M.H. Voogt
Number of pages	31 (incl. appendices)
Number of appendices	0
Sponsor	Dr. D.C. Zijdeveld, MPA
Project name	ETP Modelling
Project number	043.01048
Postscan number	TNO-060-UT-2013-00295

All rights reserved.

No part of this publication may be reproduced and/or published by print, photoprint, microfilm or any other means without the previous written consent of TNO.

In case this report was drafted on instructions, the rights and obligations of contracting parties are subject to either the General Terms and Conditions for commissions to TNO, or the relevant agreement concluded between the contracting parties. Submitting the report for inspection to parties who have a direct interest is permitted.

© 2013 TNO

Contents

1	Introduction.....	3
2	Program description	4
2.1	Rationale of the ETP Modelling	4
2.2	Vision	5
2.3	The three modelling challenges.....	6
3	Midterm results	10
3.1	Modelling socio-technical systems	10
3.2	Bridging scale levels in Fluid and Solid Mechanics.....	15
3.3	Increasing applicability: robustness, validity, accessibility, speed	22
4	Signature	31

1 Introduction

This report has been prepared for the Midterm Review of the Enabling Technology Program (ETP) 'Modelling'. This 4-year TNO research program started in 2011. The report presents a description of the program along with a summary of results that have been achieved in 2011 and 2012. It is based on the annual reports 2011 and 2012.

2 Program description

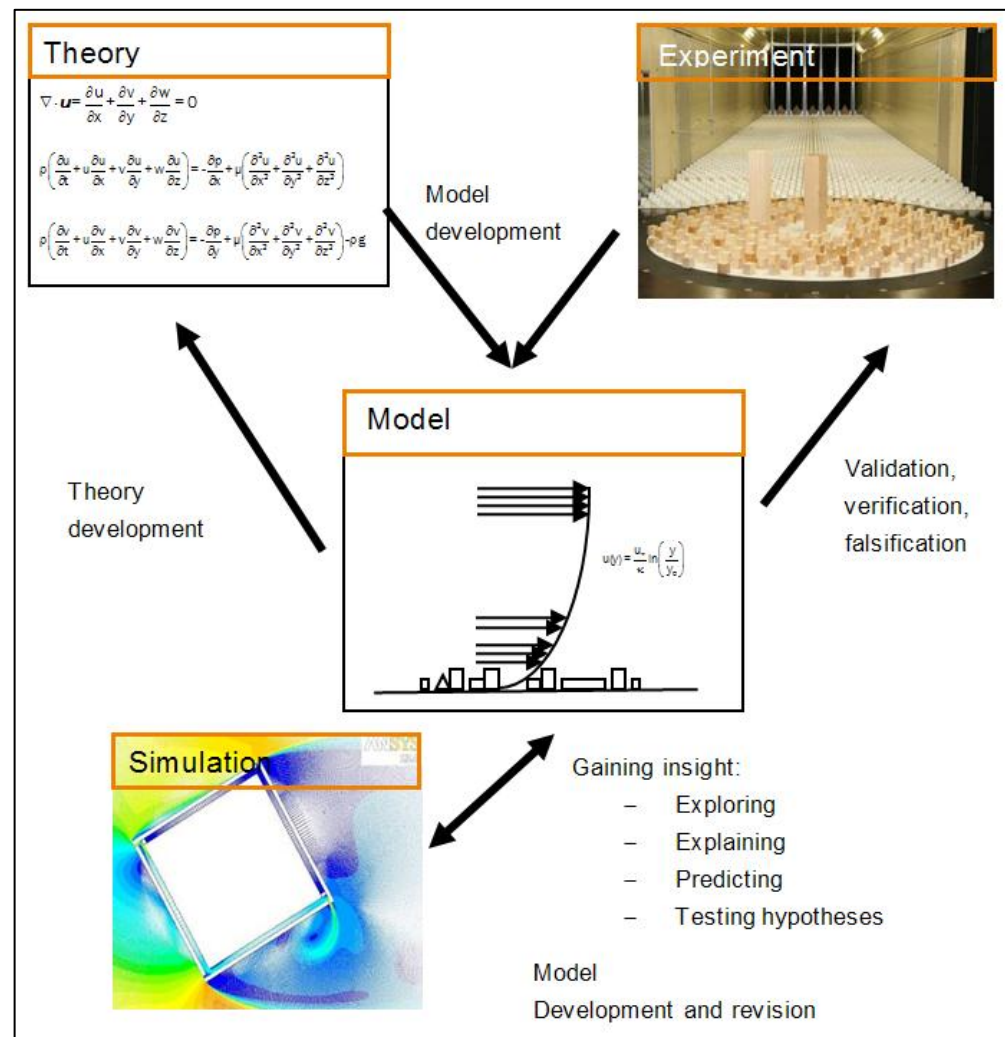
2.1 Rationale of the ETP Modelling

Models are of central importance in many scientific contexts. The centrality of models such as the billiard ball model of a gas, the Bohr model of the atom, the double helix model of DNA, agent-based and evolutionary models in the social sciences, or general equilibrium models of markets in their respective domains are cases in point. In short, models are one of the principal instruments of modern science. They allow for complete freedom to test hypotheses, to explore all implications of theories, to evaluate possible solutions and to predict outcomes of scenarios. In doing so, experts continuously revise and adjust their models according to new insights; as such models are to be considered as knowledge repositories.

Models facilitate the translation from science to practice as they form an excellent means to disseminate knowledge to a wider audience. Since a model is a repository of knowledge, model simulations can mediate this knowledge by presenting results in an instructive and intuitive manner. Something theories, often mathematical abstractions, cannot provide. This mediation of knowledge enables us to interact with the reality the model describes: simulations provide necessary information in an interactive way for decision and policy making, or simulations can directly interact with reality, for instance in an industrial control process or in a design process.

Taking all these features combined, a model is a tool with the following functions:

- Knowledge function: Increase understanding, explaining, verifying, exploring, predicting;
- Informative function: Transfer of knowledge to a wider audience;
- Interactive function: Control, design, and decision making.



An example of a model and its relations with theory, experiment and simulation. The picture reveals the interdependency of all elements. The example here is the atmospheric boundary layer.

2.2 Vision

In the value chain TNO has the role of innovator, meaning TNO intermediates between academic knowledge development and societal and technological needs. Models play a crucial role in enabling TNO to bridge the gap between academia and application. This becomes clear when we rephrase the general features of models in terms of needs for TNO. Models constitute a critical success factor for TNO, since:

- **Models are tools for knowledge management** As repositories of knowledge; academic models form an excellent and efficient means of transferring knowledge. Academic models form the starting point to develop practical tools, where the original model with a strictly scientific function is extended with informative and interactive functions. Without models knowledge transfer would be far more costly and time consuming.
- **Models accelerate the development of new products, services and methods** Scientifically; a better understanding enables accurate predictions that replace *trial and error* methods and time demanding experimental methods. Notably this includes life time prediction of materials, structures, and products in general. Second, exploring in simulation, although strictly speaking a *trial and error* process, is still far more time efficient than exploring with experimental methods.
- **Models enhance decision and policy making** Models transfer knowledge and enable intuitive interaction. Model simulations predict the effects of possible decisions. The possibility to explore different options will increase efficiency of collaborative processes.
- **Models reduce development costs and costs of decision/policy making** since acceleration results in cost efficiency.
- **Models enable innovation** Exploring in simulation gives a large degree of freedom, which enhances creativity. Also models integrate knowledge; as in the climate model example a model can contain different sub models. Coupling different disciplines model-wise offers the user to try different combinations. Freely exploring and trying new combinations promotes innovation and improvements.

2.3 The three modelling challenges

In order to create impact we need to utilize models for addressing societal trends, as appointed in TNO's Strategic Plan 2011-2014; demographic changes (aging), increasing mobility, (energy) scarcity, geopolitical shifts, increasing environmental pressure, etc., are all issues that exceed current traditional models abilities. We recognize the following challenges:

- 1 Modelling of socio-technical systems
- 2 Bridging scale levels in Fluid and Solid Mechanics
- 3 Increasing applicability: robustness, validity, accessibility, speed

It is the ambition of TNO to have an acknowledged European top position on modelling of societal and technological issues. That is why we focus on the above challenges and have dedicated an Enabling Technology Program to modelling.

These challenges are described in more detail below.

Modelling of socio-technical systems



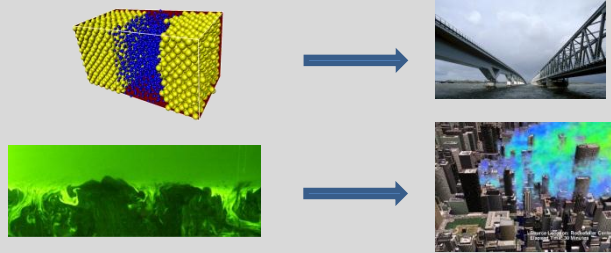
Societal and technological issues are multidisciplinary of character. Breakthroughs occur at the crossroads of disciplines. In the traditional approach modelling takes place in individual scientific fields and when applied to address a certain issue, several individual model results are combined ad hoc. However, combining results from different fields requires a well balanced analysis of the problem and the information needed. In other word issues of ever increasing complexity require a system of systems approach. Its central task is to combine models of widely differing characters, operating at different time and length scales into a valid system model.

Also, this challenge encompasses incorporation of the 'human factor'. Human activity drives societal issues and in model tools for decision making should take into account the different value orientation.

General research issues:

- Dealing with multiple perspective in decision making (policy making)
- Modelling socio economic impact
- Combining heterogeneous models; notably with qualitative and quantitative information
- Modelling human behaviour: how to facilitate the step from conceptual to simulation model
- Emergent behaviour
- Combining human factor and technical systems

Bridging scale levels in Fluid and Solid Mechanics



Fundamental knowledge describes properties at the smallest scale levels; model-wise this is the field of Fluid and Solid Mechanics (FSM). Development of academic knowledge occurs predominantly at the smaller scales (e.g. quantum, subatomic, atomic levels) where first-principle models apply. Bringing these models to the macroscopic scale of application, would provide powerful tools with optimal freedom to design new materials and industrial processes. In principle FSM models cover the entire scale range, but practically this is not feasible in a straightforward manner. Bridging all relevant scale levels requires a high-level expertise of FSM modelling, including model reduction techniques, computational speed-up techniques and coupling of models for different subdomains of physics and chemistry and for different scale levels.

General research questions

- What is the critical scale level to start from?
- Bringing the scale level of academic research to the level of application
- Uncertainty quantification
- How does uncertainty propagate through the scale levels?
- Required level detailed needed in relation the problem (model reduction)
- Coupling of different types of physical models

Increasing applicability: robustness, validity, accessibility, speed



Obviously applicability is a necessary condition of any model. However, given the aforementioned challenges applicability becomes a challenge in itself. Multidisciplinary system models involve various types of data, but need to process this data in such a way that user(s) can interact with these types of data in an intuitive manner. Also system models need to be robust under various scenarios. Models are especially useful for supporting collaborative processes, which makes intuitive user interaction even more pressing. In addition it requires model responses to be sufficiently fast to interact with. The human factor can be modelled based on expert-judgment or surveys, which poses serious questions on general validity. Bridging scale levels requires sufficient accuracy and validity at the small scale to produce meaningful, statistically significant results at the application level. In order to explore and predict computation speed is important, and even essential in control processes.

General research questions

- Speeding up simulations with hardware
- Architectures for flexible coupling of models, data, sensors
- Model reduction (strongly related but not necessarily limited to physical modelling)
- Reducing uncertainty and increasing predictive power
- Visualisation of uncertainty
- Interacting with complex 3D,t (simulation) data

3 Midterm results

This report primarily presents the progress of the ETP in broad outline. The results are organized along the four challenges of the ETP. For each challenge the main results are highlighted in the grey boxes, followed by more details for each result below the box.

3.1 Modelling socio-technical systems



1. **Structured and transparent decision making with models.** Multiple perspectives, combining quantitative and qualitative information (of different types of risks), eliciting values of multiple stakeholders, prioritizing risks in a comprehensive model system enables structured and transparent decision making in a cost efficient manner of complex societal problems. Developed in this ETP 2011-2012 and will be applied in a project for the United Nations Interregional Crime and Justice Research Institute.
2. **Better policy making in socio-economic problems: social return case.** New policies have long term socio-economic effects with possibly counter-effective outcomes. A novel combination of system dynamics and value network analysis enables decision makers to anticipate on these long term effects as this model approach reveals how measures propagate through the system and affect the interest of different stakeholders. This will lead to better and more informed policy making. The model approach is tailored to the social return case and will be applied in 2013.
3. **How do my eating habits influence the chance of developing type 2 diabetes?** Food and sleeping habits, exercise; all qualitative of nature but interact with metabolic quantities such as insulin sensitivity and tissue damage. In a system dynamics modelling approach these qualitative and quantitative factors are combined, revealing how these factors interplay. This model enables non-medical specialists to understand the effects of behaviour on the human body health.
4. **Reliable smart grids and impact of failure: linking technical social-behavioural and impact models.** We have developed a model that connects technical networks, human-factors and cost-benefit analysis of a smart electricity grid, so that the different components interact, allowing for simulation of future events. As such, it becomes possible for the first time to investigate a number of what-if scenarios whilst taking into account the various technical and social factors and their interdependencies. Such a model strategy enables policy making for vital infrastructures, such as smart grids.

1. Structured and transparent decision making with models

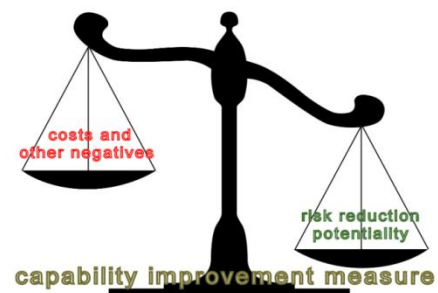
Structured and transparent decision making and/or devising successful (policy) interventions in the dynamics of our society require more than ever dedicated complex modelling capabilities. Therefore, the goal of this project is to develop a system of systems analysis and design modelling approaches to:

1. achieve insight into the structure of a system of systems and underlying relations and
2. enable informed, systematic and transparent decision making.

The methodological work on multi-perspectives started in 2011 and was completed in 2012 resulting in a multi-methodology approach that:

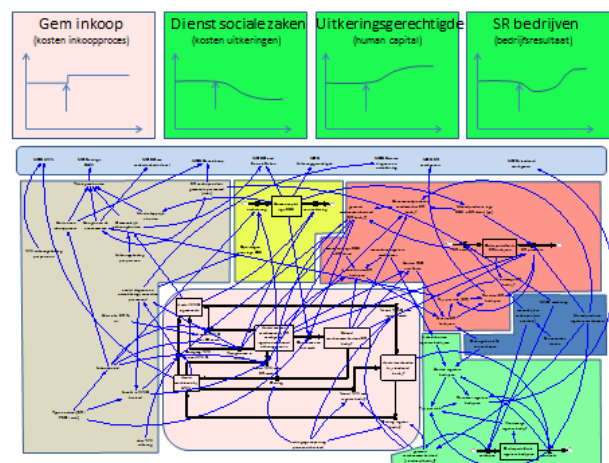
- Assesses and compares different types of risks
- selects those that are more serious than others
- prioritises measures that could bring about capability improvements,
- combines quantitative and qualitative information in a novel way,
- elicits stakeholders values regarding impact of risk in a novel way,

and thereby spend a limited budget as effectively as possible, whilst taking the human factor into account. As such this multi-methodology is suitable for application by (inter)national, regional and local government bodies, emergency service authorities and large companies dealing with risks. As for 2013 this multi-methodology will be used in a project conducted for the United Nations Interregional Crime and Justice Research Institute.



2. Better policy making in socio-economic problems: social return case

A new socio-cost modelling methodology was developed to model the propagation of socio-economic effects of innovations for different stakeholders for a given system. This methodology combines Value Network Analysis and System Dynamics and was applied to a hot topic in the Dutch society, social return.



Social return concerns development of agreements related to employment and internships in procurement of services, works and supplies. In a social return agreement the contractor, when performing the contract, promises to create jobs, internships or workplaces for a certain number of people with a distance to the labour market, low education or disabilities. In the case study the introduction of social return is considered and the (socio-economical) effects for all stakeholders

are analysed. We have applied the new methodology for the case of the 'traditional' form of social return as well as for the case of applying social return, in combination with the TNO tool Performance Ladder Inclusive Entrepreneurship (PSO: *prestatieladder socialer ondernemen*).

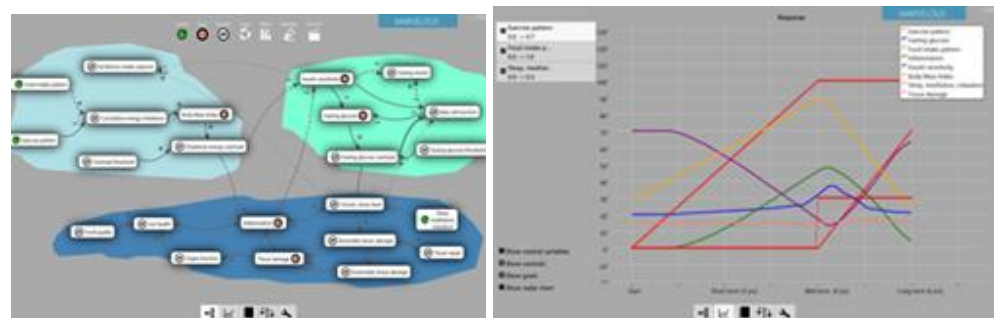
Traditional social return requirements are typically tied to a specific contract and therefore only hold for the duration of this contract. This limits the actual contribution to the development of human capital of the social return candidates. Also, the current social contribution of companies, i.e. providing employment for disadvantaged groups, is usually not taken into account when evaluating the tenders. This is disadvantageous for employers that already provide much employment for vulnerable groups and may even lead to dismissal of current employees to be able to meet the new social return requirements. To stimulate sustainable employment for disadvantaged groups, TNO developed the Performance Ladder Inclusive Entrepreneurship (Prestatieladder Socialer Ondernemen (PSO)) for measuring the extent to which companies contribute to the employment of vulnerable groups. The PSO accounts for both the quantity and quality of the employment for disadvantaged groups. The PSO can be used as a tool for social return in procurement.

With our new methodology we are able to analyse what the effects of both traditional social return as well as applying social return with the PSO are for the various stakeholders (municipality, employers and the unemployed). This helps policy makers to make better decisions on which form of social return they should use. Ultimately this will lead to more effectiveness in terms of higher employment and increased productivity.

Our new multi-methodology is ready to be tested in 2013 on the social return pilot, with the use of the PSO, of the municipality of Apeldoorn. The generic method is suitable to evaluate the socio-economic effects of a new policy or new technology and will be further tested in 2013.

3. How do my eating habits influence the chance of developing type 2 diabetes?

Modelling strategies to combine qualitative and quantitative factors were explored in close cooperation with ETP System Biology and resulted in the development of a first prototype of a systemic health model for the development of type 2 diabetes.

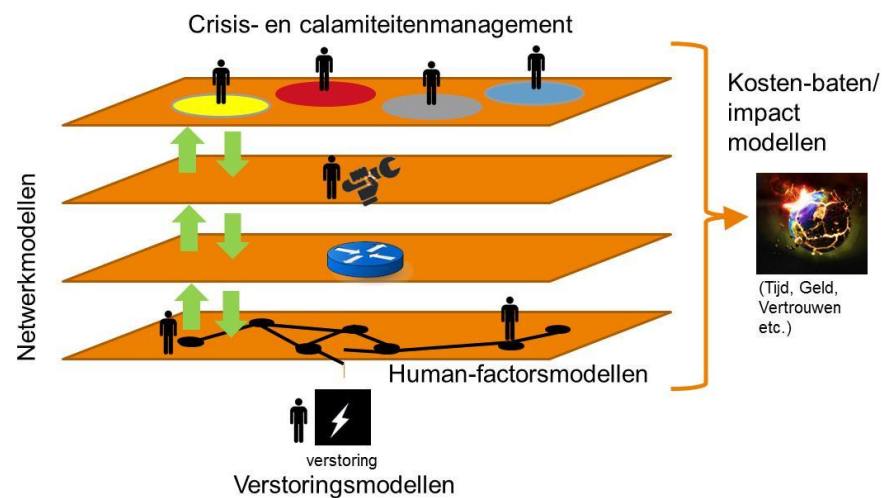


This model has been implemented in TNO's system dynamics model MARVELous and models the different effects of human behaviour, like eating too much food, not having enough physical exercise, lack of sleep on human body health, like the body mass index, insulin sensitivity, inflammation and tissue damage. This model enables non-medical specialists to understand the effects of behaviour on the

human body health. After validation, it might be used by doctors, dieticians and teachers to convince patients and students to change their behaviour and as such to prevent the development of diabetes type 2.

4. Reliable smart grids and impact of failure: linking technical, social-behavioural, and impact models

We have developed a model that connects technical networks, human-factors and cost-benefit analysis of a smart electricity grid, so that the different components interact, allowing for simulation of future events. As such, it becomes possible for the first time to investigate a number of what-if scenarios whilst taking into account the various technical and social factors and their interdependencies.



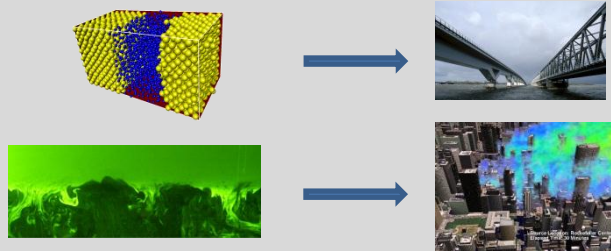
A major frontier in understanding the changing nature of society is to link models of novel infrastructures, such as smart electricity grids, with behavioural models of the those who will actually be faced with using the new systems and also with impact models of the costs and benefits to society as a whole. The advantages of creating valid, interdependent network models are significant: allowing for better planning, more focused technological investments, and speeding up societal acceptance of large-scale innovations.

The new model (first applied to smart grids, but applies to networks in general) takes account of short term fluctuations, such as a power-management application switching on a freezer, as well as long-term changes, such as shifts in people's attitudes about solar power. This has been achieved by bringing together expertise on consumer behaviour, sociology, network modelling, electricity grid topology, cost-benefit modelling and multi-agent simulation modelling.

A significant improvement on previous models of separate infrastructures or network models of individual domains, this new interdependent socio-technical model allows us to explore complex uncertainties with important implications for next-generation infrastructure developers and policy makers. For example, when decentralized, renewable energy production becomes dominant and price variation is introduced to encourage consumers to use more electricity at times with favourable wind condition; how will people react? Could a behavioural cascade, such as preferred settings in a power-management application, lead to a failure cascade in the electricity grid? What are the longer-term implications for the stability

of the electricity network if government subsidies for solar power are increased?
And, what are the costs to society of low-chance, high-impact disruptions, both economically and in terms of trust in the new infrastructure?

3.2 Bridging scale levels in Fluid and Solid Mechanics

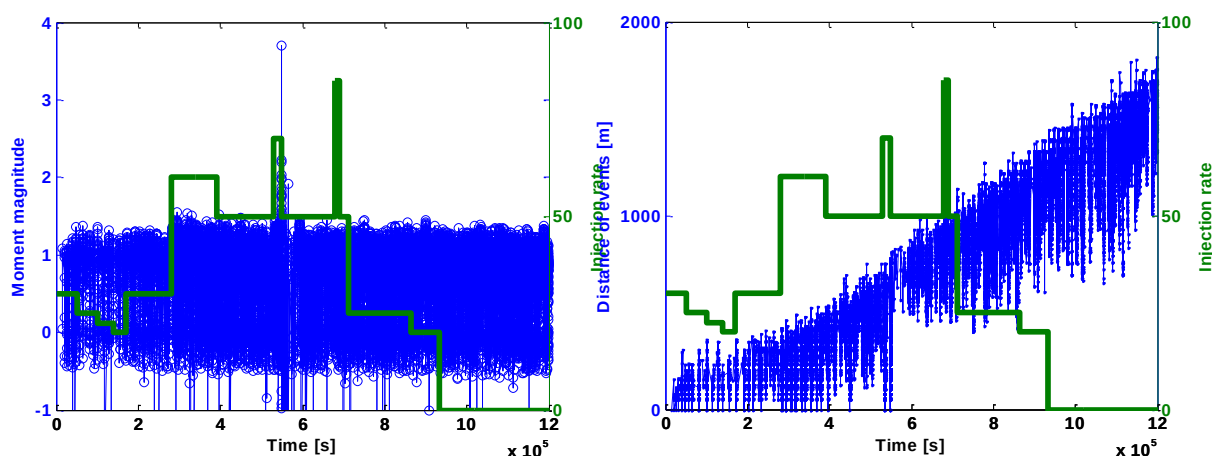


5. **Enhancing geothermal energy production and reducing risks.** Extracting heat from deep subsurface reservoirs relies on opening fractures by pumping water into the reservoir. This year we developed a model for fracture reactivation. Such a model enables optimization of geothermal energy production and reducing associated risk. Reactivating fractures implies causing seismicity. So while induced seismicity is necessary for geothermal energy production, it is also a risk. First results show good agreement with observations, so an important first step has been taken towards model-based support for geothermal production.
6. **Model-based fast up-scaling of novel chemical reactor types: TNO helix reactor.** New models have been developed to optimize new prototypes of chemical reactors. Validated with a lab-scale reactor prototype, the model enables optimization of the prototype and subsequent up-scaling to the scale of real application. This achievement makes time-consuming and costly experiments redundant.
7. **“FaiMoS” for accurately predicting failure of large structures.** Structures need to be safe, reliable and sustainable, but at acceptable costs. Damage is nearly always initiated at discontinuities in the structure such as welded joints. Solutions are sought by improving models, increasing numerical efficiency and connecting structural behaviour to microscale physics. A framework for different materials and failure mechanism is being built up.
8. **Reliable simulations of hazardous heavy gases.** Releases of heavy gases such as CO₂ and LNG are hazardous for health and environment. With transitions in energy sources and climate mitigating measures such as CCS, the risks need to be assessed. Especially for the built environment, reliable models were lacking. We developed CFD models that agree well with validation data from field and wind tunnel tests.
9. **Realistic, but higher levels of pollution due to thermal effects in the atmosphere.** A new model for the atmospheric flows that takes into account thermal effects shows that vertical motions are suppressed, leading to much higher concentrations of pollutants than calculated with conventional models.
10. **Durable protection of decorative coatings.** The development of models for transport in permeable materials enables applications in various fields, ranging from coatings, concrete, geothermal energy production and food. In that framework a model has been developed that accurately predicts the controlled release of protective chemicals and biocides in coatings, and enables to design waterborne coatings with sufficient protection.

5. Enhancing geothermal energy production and reducing risks

Geothermal Systems can be used to extract heat from deep subsurface reservoirs to produce electricity. Enhanced Geothermal Systems rely on the stimulation of the deliverability (the heat production) through the opening of fractures by pumping water into the reservoir under high pressures. The opening is achieved using fracture reactivation and may consequently induce seismicity. The seismicity is necessary for the reactivation, but at the same time it is a risk.

Modelling fracture reactivation and the associated seismicity is critically dependent on coupling multi-physics: flow, mechanics and heat. We developed a coupled code to obtain a better understanding of the role of the water pressure changes in the reservoir that cause fracture reactivation and seismicity. Using this code we created a model inspired on the Soultz-la-Forêts GPK3 injection well, intersected by a dominant fracture zone. The model reproduced reactivation of the fracture zone and we observed the growth of a zone with large directional permeability.



The left figure presents model results of seismic events and the correlation with the injection rate. Many small events and some large events were predicted. The right figure shows the corresponding development of seismicity in time and space. The area in which seismicity is observed moves away from the injection point, as had also been observed in the actual field test.

Our model helps us in understanding the stimulation performance and the induced seismicity as observed in the field test. It will also help in making better designs for new stimulation treatments by facilitating better forecasts for heat production and better assessments of risks due to induced seismicity.

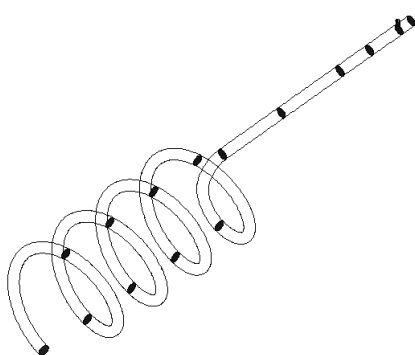
6. Model-based fast up-scaling of novel chemical reactor types: TNO helix reactor

Numerical simulation with Computation Fluid Dynamics (CFD) allows predicting the trend of the flow variables in single and multi-stage reactors in chemical process engineering. This enables a model-based up-scaling from reactors in a laboratory set-up to plant-scale and reduces the amount of costly experiments.

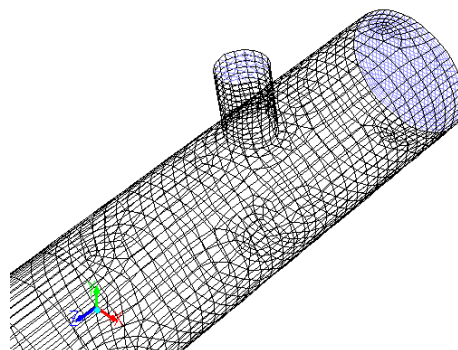
Process intensification is strived for in chemical process engineering in order to achieve substantial improvement on the performance of the process plants. The TNO helix reactor is a process-intensifying, innovative reactor which encourages homogenous mixing of chemical substances.

Mixing of flows of different phases (gas-fluid-solid) has proven to be difficult to simulate numerically. Numerical instabilities can arise due to rapid mixing of two immiscible-like inflows with a high viscosity difference. In this work, the CFD capability of modelling mixing is thoroughly investigated for an acid stream being neutralized by a basic stream in a Helix reactor (see Figure). Mixing processes of fluid-solid mixtures in other types of reactors (the oscillating baffle reactor, wash column) were studied as well. It is demonstrated that the simulated results show a good agreement with earlier experimental observations.

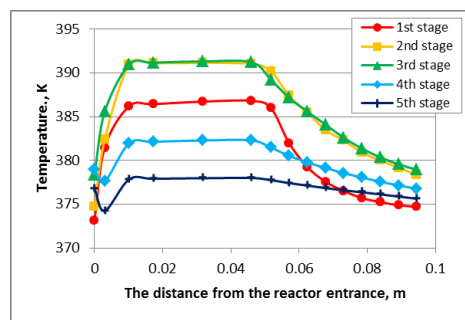
For all types of reactors it can be concluded that the inflow conditions are very important. Without the proper inflow conditions completely different processes and flow regimes are found. Another important aspect is the model chosen for particle transport. The best model turned out to be the Eulerian-Granular model, however special care has to be taken for the boundary conditions since the standard conditions do not apply.



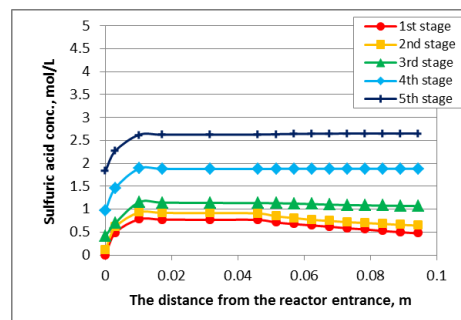
(a) Helix reactor



(b) Numerical grids at the entrance of the feeding tube.



(c) Temperature [K]



(d) Sulphuric acid concentration [mol/L]

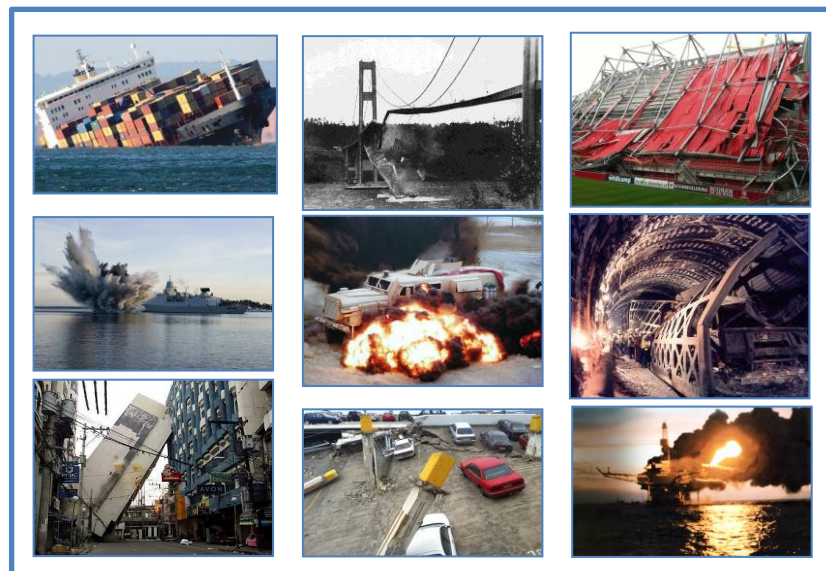
7. FaiMoS for accurately predicting failure of large structures

FaiMoS (Failure models for large structures) improve lifetime of structures and operational reliability, enable safety, durability and cost reduction by improving the key issue that falls short in nowadays prediction models: **failure**.

Failure prediction often needs very detailed analysis. The level of detail can become as small as nm conflicting with structural dimensions that can be up to tens of meters. Its combinations can result in computing times in the order of years. Solutions are sought by improving models, increasing numerical efficiency and connecting structural behaviour to microscale physics.

Examples of current developments are:

- A replacement element with plastic and failure relations. This element replaces the need for a highly detailed (thus, time consuming) mesh for joints in larger structures.
- Predicting failure in crashing and forming of “thin-walled” metal structures such as ships, is made available by deriving a relationship for failure strain with state of stress and element size.
- A course modelling technique for debonding failure for fibre reinforced materials in out of plane loading enables analyses of car impact onto composite bridge structures, assessments of the effects of slamming on ships and explosive loadings on structures such as ships or blast walls.
- A model that simulates fatigue crack growth in and near welds in metal structures being able to simulate load-sequence effects, such as crack retardation following a large load cycle. This can extend life time of structures such as bridges and wind turbines.
- A multi-scale FE framework that allows to incorporate the micro- and/or mesostructural material response in macroscopic FE models, in order to improve material modelling including failure initiation and damage evolution of heterogeneous materials.

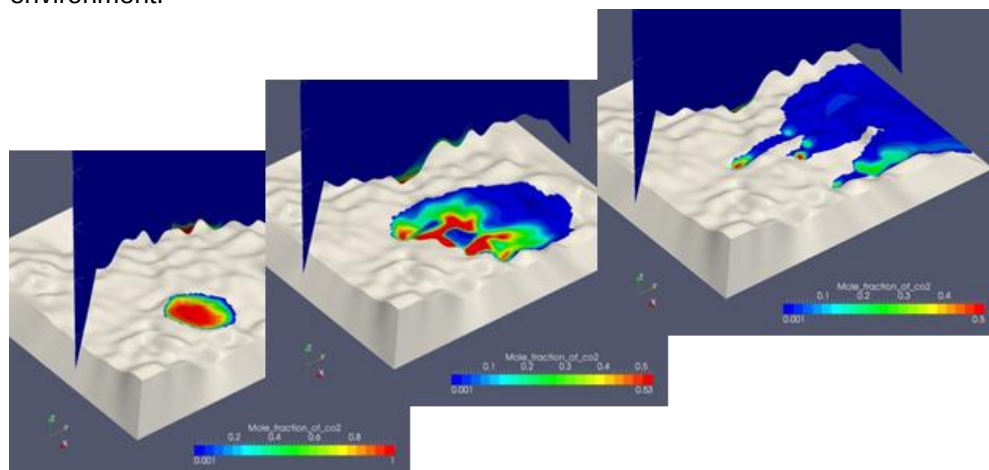


8. Reliable simulations of hazardous heavy gases

At industrial but also public sites, with road, train or ship transportation, industrial gases or liquids with heavy gas behaviour are stored commonly in quite large amounts. If being released by accident, the dispersion of these gases is driven by gravity which makes them flow with a comparable behaviour to water. Since cavities, depressions or lower levels might be filled with these heavy gases, the effects distances in the case of a hazardous release have to be predicted accurately. Heavy gases are e.g. LPG or CO₂, but also gases lighter than air like LNG or Ammonia show heavy gas behaviour since they are usually released in a liquid and gaseous state at low temperatures. LPG and LNG are or will be stored in large amounts at filling stations, or are transported by road, train or ship. Ammonia is used in large amounts in the fertilising industry and many buildings like parking garages or industrial sited have CO₂ fire extinguishing installations where up to 20.000kg of CO₂ might be released accidentally. Not only the inside of these

buildings are affected, but also the venting of the buildings after the incident might have catastrophic effects.

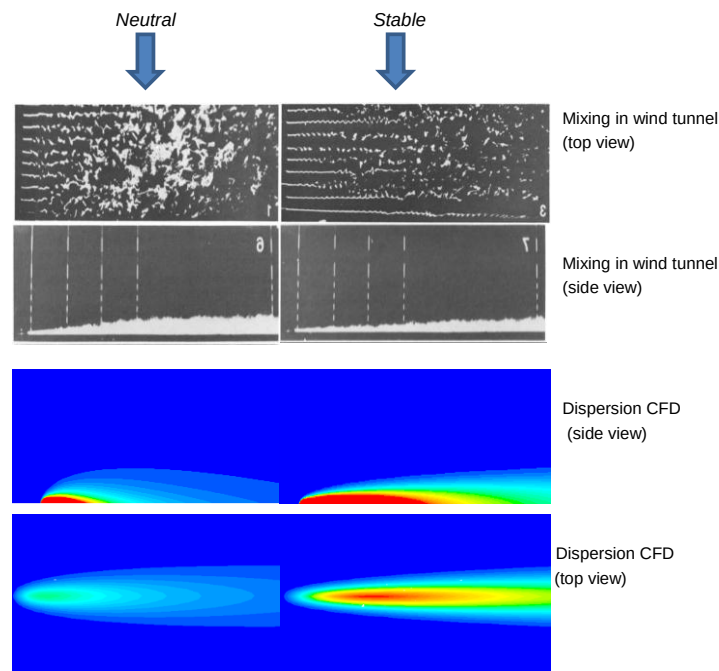
TNO has been working not only to match experimental data with the numerical CFD (Computational Fluid Dynamics) modelling but also to separate and investigate the contribution of the different physical effects involved. By analysing many experimental data and rebuilding them numerically, the different effects like inducing turbulence at the boundaries of the heavy gas, the immediate damping effect due to the released heavy gas and the interaction with the turbulence present in the surrounding atmospheric boundary layer were separated. The numerical results are in excellent agreement with experimental data from experimental tests for internal flows, wind tunnel testing (including terrain effects, the built environment and atmospheric boundary layers) and field experiments. In the Figure below, a CO₂ pipeline rupture scenario in a hilly, sloping terrain is shown. For heavy gas, slight changes in surface topology (1-2m) are sufficient to change the dispersion pattern significantly since depressions are filled rapidly with heavy gas but vented is very slow. In the present case, the dispersion pattern differs significantly from the well known Gaussian dispersion pattern with respect to space and time which makes the CFD models an excellent tool to predict heavy gas dispersion in complex environment.



CO₂ pipeline rupture scenario with dispersion of CO₂ in a hilly, sloping terrain. Effect distances of up to 1.5km a timescales of 1500s appear. (times at 75s, 320 and 1000s)

9. Realistic, but higher levels of pollution due to thermal effects in the atmosphere

Temperature effects in the lowest levels of the atmosphere can create a stable boundary layer in which vertical movement is suppressed. For air pollution or a release of a hazardous substance, this constitutes a worst case situation with very high concentrations. Current models neglect such thermal effects, called neutral stability. In the ETP a model has been developed that simulates a stable thermal boundary layer and has been validated with wind tunnel experiments. The figure below shows wind tunnel experiments and CFD simulations for a neutral and stable case. Both in the wind tunnel and the simulations the mixing is suppressed during stable conditions, leading to higher concentrations.



10. Durable protection of decorative coatings

Permeable materials form the basis of the built environment (e.g. concrete, cement, stone, plasters, and coatings), and deep subsurface (sandstone, clay, limestone, etc.). More specifically aging of building materials threaten the safety, usage, comfort, and health of the users. The costs necessary for maintenance and repair are high, in terms of money, energy and raw materials. In the deep subsurface transport is crucial for the application of geothermal energy. Models form the basis for this understanding and controlling the complex processes in materials and objects. In the above sketched cases the general element is transport. However, currently many existing models only account for transport of one component, and are generally not multi-components (e.g. water and soluted substances), nor multi-physics and account for subsequent reactions like solubility, crystallization and release. Furthermore, most models focus only on one length scale. Consequently, we need to focus on developing new state-of-the-art models.

The potential of such models is illustrated for the application of coatings. Decorative coatings usually require the addition of dedicated bio-active chemicals, i.e. biocides, to increase their bio-resistance and thus reduce the growth of algae, fungi and bacteria. These additions are necessary since micro-organisms (i) induce biodegradation, which negatively affect the durability of materials, (ii) affect their aesthetic value, and (iii) cause unhealthy indoor environments. The risk increases rapidly since the market focuses more and more on waterborne coatings. For the above reasons, new technologies are currently developed within TNO to reduce the biocide concentration in materials and prolong their protection. However,



implementation of these technologies is difficult since the knowledge of the fundamental processes that determine biocide release is lacking. Consequently, a model has been developed which describes the release of biocide. The model developed in 2011 can predict the complex release behavior in a gypsum substrate (model system) on the basis of the main processes, which are characterized by parameters such as diffusion, and solubility. Based on the parameters, which can be obtained from simple and fast experiments, an accurate prediction can be made of the behavior in the final material. Moreover much more insight has been obtained about which processes are dominant in this situation. In 2012, a transport model for coatings was developed. This second generation model contains three basic processes. These are uptake of water in the material, dissolution/recrystallization or release/binding (e.g. induced by water), and subsequent transport to the surface. After model verification and investigating the behavior of biocide release for combinations of these three processes, the model was used to simulate a so called rain test with alternating wetting and drying cycles. A difference in release was found, which in this case is caused by changes in the chemical equilibrium (e.g. dissolution). The next steps are to simulate the release behavior of biocides in different situations, and understand the implications of the model in practical situations (e.g. compare it to outdoor weathering). To do that some input parameters are needed, than can be obtained using simple experimental methods.

3.3 Increasing applicability: robustness, validity, accessibility, speed



- 11. Data assimilation enabling CO2 capture and storage.** In CO2 capture and storage (CCS), the most important source of uncertainty is the geological structure and the distribution of facies in a reservoir. Instead of utilizing traditional approaches, we adopted a stochastic approach by looking at the probability of the existence of a certain type of facies. This gives a highly reduced model that is projected in the space of probabilities. Next year this method will be applied to a real field case, the Norne field. This method is generally applicable to problems with categorical variables.
- 12. Sensators.** Objects that interact with multiple users through sounds, lights, forces and vibrations and can move autonomously. They provide a new way of interacting with complex simulation systems. A patent request has been filed.
- 13. In practice: multiple stakeholders decision making with models.** Together with expert end-users, an integrated demo was developed to show the use of 3D models, visualizations and tangibles in a multiple stakeholders decision making process. The demo was on the 'sand motor case'. In this case animations of water currency models (delivered by Deltares) were used.
- 14. How to present uncertainty to non-experts.** To investigate whether perceived uncertainty is affected by the type of visual uncertainty representation, we tested how non-experts judge point probability for seven different visual representations of uncertainty. The results show that perceived uncertainty depends both on the visualization type and on the observer's numeracy.
- 15. Software Framework completed and applied** The IBM framework to combine complex models, sensors and data in a single simulation system has been finalized. The wide range of use cases proved the large flexibility of the framework: remote sensors data from the Orleans building connected to simulation software, an embedded control device for concert halls and interconnecting Urban Strategy with Phoenix (Geodan software).
- 16. Accelerating traffic noise simulations** with video cards in regular PCs providing the general audience simulation times that would normally require an advanced supercomputer. A model for traffic noise has been accelerated 250 times.
- 17. Accurate and fast simulations of blasts impact on structures.** A method for calculating the effects of blasts on structures that gives accurate results in several hours. Previously, either the simulation time (> 1 year!) or the accuracy was unacceptable.

18. Update your beliefs in order to simplify empirical models and reduce uncertainty. With graphical Bayesian Networks we are able to reduce the number of variables in a model and reduce uncertainty. We have shown how this method helps simplifying the calculation of wind loads on a building from wind tunnel experimental data.

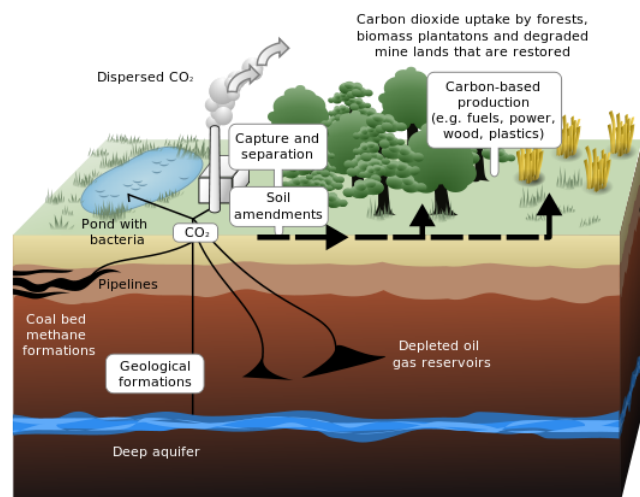
13. Data assimilation enabling CO₂ capture and storage

The target of data assimilation is to combine model simulations and observations into a merged product with higher accuracy. Data assimilation is applied in a large range of applications, from fine scale control of industrial production processes, to large scale geophysical applications such as weather forecasts and oil exploration. Although the applications are different, data-assimilation techniques share the same ingredients: model simulations, observations, and uncertainty descriptions. The general philosophy that guides the development of the ETP Data Assimilation project is based on the idea that research should be done with a certain application in mind, and vice-versa: the problems encountered in the real life application should generate more theoretical questions for the fundamental research. On a top of this cycle we should have available a general framework, a tool, which can be easily used in different applications and with different methods and algorithms fit for the purpose in hand.

In CO₂ capture and storage (CCS), the most important source of uncertainty is the geological structure and the distribution of facies in a reservoir. Instead of utilizing traditional approaches, we adopted a stochastic approach by looking at the probability of the existence of a certain type of facies. This gives a highly reduced model that is projected in the space of probabilities. Next year this method will be applied to a real field case, the Norne field. This method is generally applicable to problems with categorical variables.

Although CO₂ has been injected into geological formations for several decades for various purposes, including enhanced oil recovery, the long term storage of CO₂ is a relatively new concept. The first approach is in an initial phase (experimental) of implementation in a real field case of CO₂ storage: "Sleipner". The most important source of

uncertainty is the geological structure and the facies distribution in the reservoir. The approach that we are usually using for handling, propagating and reducing the uncertainties is not fitted for the estimation of categorical variables (facies type 1 or 2). Therefore, a new parametrization was developed where one is looking at the



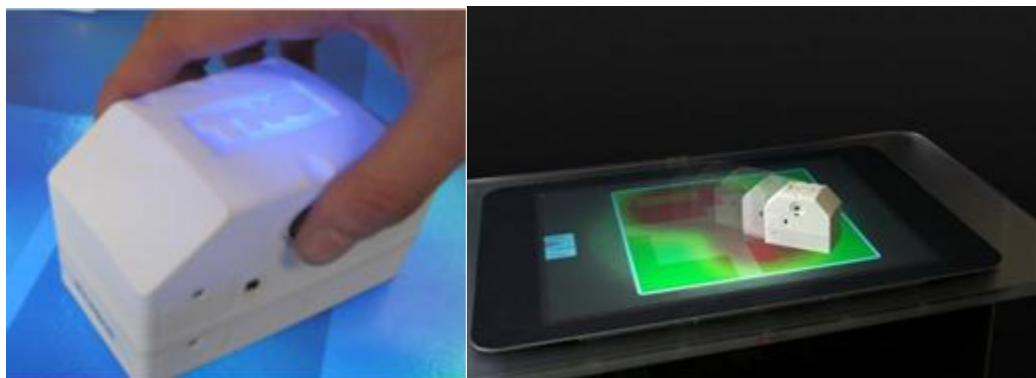
probability of the existence of a certain type of facies in the reservoir. This reduces the model by projecting it in the space of probabilities. The estimation of geological features are of high interest in order to have a safe and controlled CO₂ storage. The plans are to implement this approach in the only real field case in the reservoir engineering world open for research, the Norne field. This will be of international recognition for TNO, the results being presented at an SPE Conference in June 2013.

14. Sensors

Many of our societal challenges are complex and multidisciplinary. Involvement of multiple stakeholders in an early phase of the design and decision process is required to solve these issues. Models that predict the effects of specific design choices are becoming an important support tool. The success of these support tools depends on their user-friendliness for both experts and laymen. If the support tool is too complex to handle, we cannot achieve our goals with respect to gaining insight, transferring knowledge, exploring solution space and designing applicable results.

A single-user workstation with keyboard and screen does not allow users to get a grip on large amounts of complex, multidimensional information. Therefore, we are working on a new generation of user-system interaction interfaces that is intuitive to use and optimally facilitates creativity and collaboration among multiple stakeholders in the design and decision process. An example of such an interface is the multi-touch surface table, introduced in 2007. Surface tables facilitate users to work together in the same information space and they allow intuitive manipulation of objects through the tangible interaction metaphor. Previous experiments showed the potential of this interface but also revealed shortcomings. For instance, the interaction is rather poor in the sense that only visual information is presented as output to the user and only finger motions are used as input from the user. In the project intuitive user interaction, we develop new technology to overcome these shortcomings and further improve surface table interaction.

The figure below depicts one of the active table top prototype objects developed within this ETP.



The active objects are able to deliver direct feedback through sound, light, forces, and vibration. Furthermore, the objects can move autonomously for instance based on model output. So, imagine that the active object represents a school in an urban planning project. Urban planning models of e.g. noise and safety are constantly calculating the results of design choices and can interactively present whether the solution meets specific requirements. Stakeholders finding a good location for the

school will experience larger resistance when they move the school to a location that does not meet the requirements.

This gives them direct and intuitive feedback of the model output. Also, as soon as other changes to the planning result in exceeding the requirements, the school object can signal this actively by changing color, producing a warning signal, or ultimately by moving by itself to a new location that does satisfy the requirements. A patent application for this interaction concept and technology has been filed Sept. 2011.

15. In practice: multiple stakeholders decision making with models

Together with expert end-users, an integrated demo was developed to show the use of 3D models, visualizations and tangibles in a multiple stakeholders decision making process. The facilitation of the process is supported by a facilitator tool (presented on a tablet), that monitors the meeting and intervenes when needed. The team work is supported by a multi touch table showing a map of the environment, giving access to situational data, models and other information. Tangibles were demonstrated as a potential interaction tool. On large screens additional relevant information was shown. Also, a video connection can be made with a distant expert. The concept supports collaborative brainstorm and decision making processes.

Special software was developed for user interaction with the visualizations on the table and the interaction between the table and the other hardware. We applied the demo on the 'sand motor case'. In this case animations of water currency models (delivered by Deltares) were used.



A virtual facilitator monitors and supports the group process.



The Multi touch table allows multiple users to interact simultaneously.



Tangibles can be used on the touch table to further facilitate interaction with complex models.



Experts can collaborate (even from a distance) and use models to reach an optimal solution.

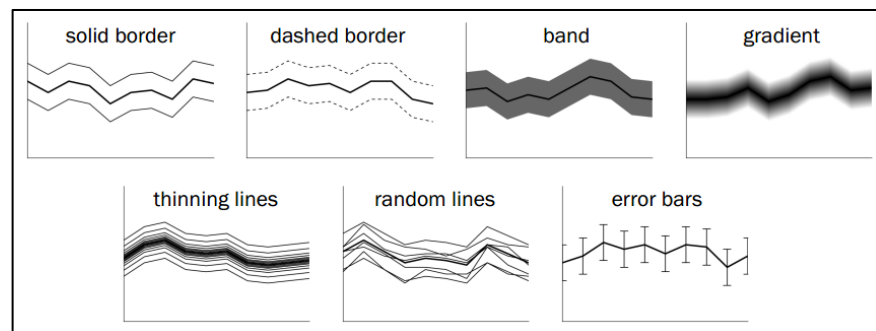
16. How to present uncertainty to non-experts

To investigate whether perceived uncertainty is affected by the type of visual uncertainty representation, we tested how non-experts judge point probability for

seven different visual representations of uncertainty (see Figure below). The results show that perceived uncertainty depends both on the visualization type and on the observer's numeracy.

For all visualizations tested, users (1) intuitively (correctly) interpreted the uncertainty range as having the highest perceived probability toward the centre of the range and lower probabilities going further outward, and (2) did not consider points outside the uncertainty range as *impossible*. However, the *random lines* visualization stood out on two aspects: (1) the results show little between-subject variability, which means that the user population (despite being quite diverse in terms of age, gender, education level and numeracy) had a uniform interpretation of the underlying probability distribution, and (2) a normal distribution best fits the results of this visualization. Hence, this representation is most suitable for a wide range of data sources with an underlying normal distribution.

Since perceived uncertainty appears to depend on the observer's numeracy, we conclude that people with low numeracy or low education level may benefit from more guidance or explanation when presented with uncertainty visualizations.



The seven uncertainty visualizations used in the study.

17. Software Framework completed and applied

The IBM framework to combine complex models, sensors and data in a single simulation system has been finalized. The wide range of use cases proved the large flexibility of the framework:

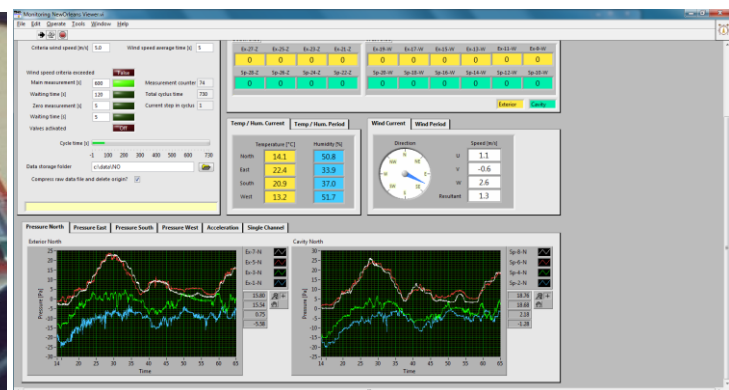
- a 'Citygame' for which a sensor (Xbox Kinect TM), image analysing models and the interactive tool for spatial planning Urban Strategy are connected. This 'game' allows the user to place ordinary 'LEGO TM' blocks to develop a new city area. The Kinect camera is used to scan the changes in the environment and uses these as input for the Urban Strategy planning instrument. Impact of changes is calculated by Fast Complex models, interconnected with the Citygame through the IMB framework. The citygame concentrates on using a 'non computer interface', making it as easy as possible for decision makers to develop different scenarios in their planning process.
- remote sensors data from the Orleans building connected to simulation software;
- an embedded control device for concert halls;
- interconnecting Urban Strategy with Phoenix (Geodan software). The generic IMB framework was used for interconnecting Urban Strategy (TNO) to Phoenix (Geodan). Phoenix is a commercial application developed by Geodan for an easy interaction with geospatial data on a MS Surface table.



Citygame overview



IMB on embedded device



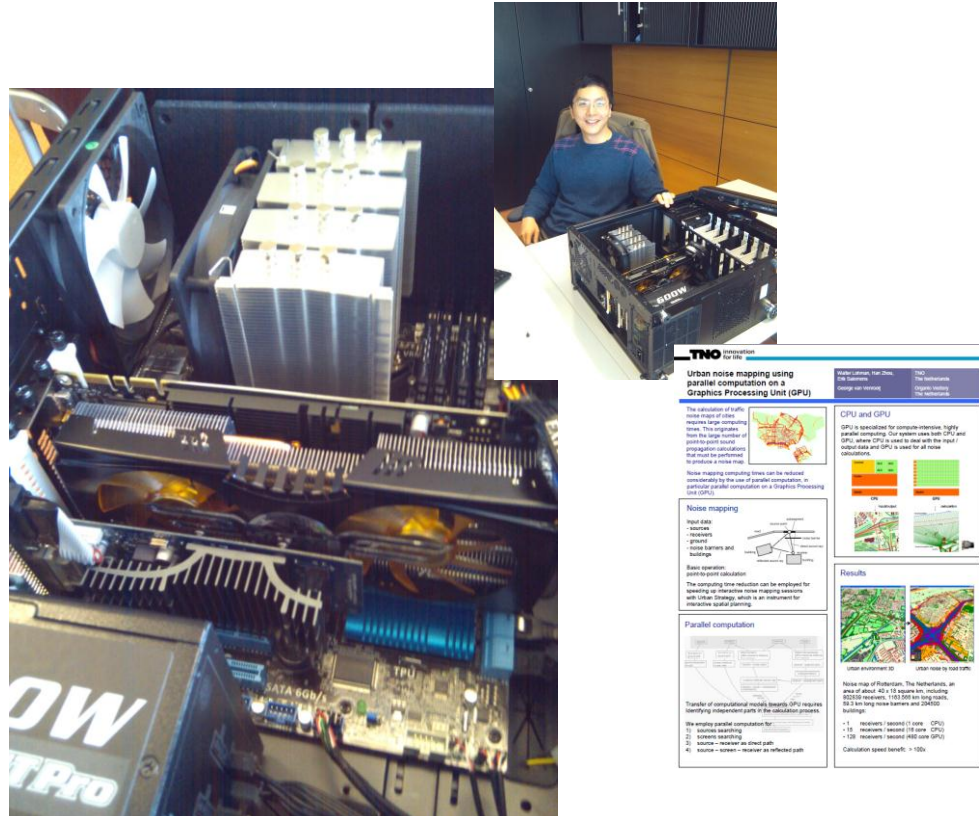
Sensor data from New Orleans building, Rotterdam



Geodan Phoenix

18. Accelerating traffic noise simulations.

High speed simulations have been achieved by utilising video cards. The GPUs (Graphical Processing Units) have a large quantity of individual processors that can operate in parallel. Normally these processors are used to do the complex 3D operations used for the recent high-tech computer games. However these processors can also be used to perform calculations of computer models that have a large demand for computational power.



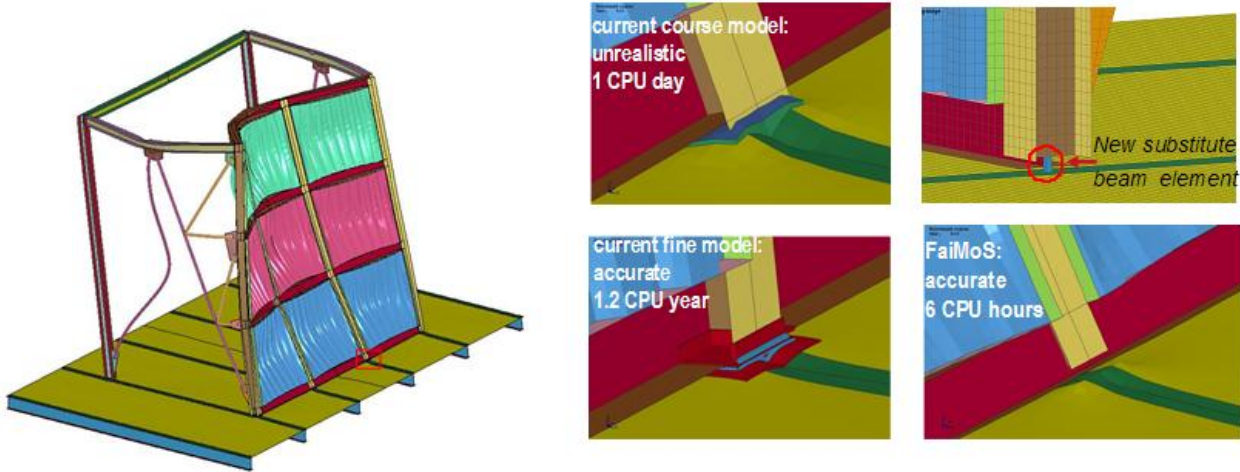
Using NVidia GTX 580 for more power!

A successful transition was made to redesign the Dutch noise model for road traffic towards the NVidia GTX 580 thus utilising the full amount of 580 CUDA processors to perform noise mapping. A poster describing the technology used won a prize at the High Speed Computing convention in Hamburg 2011. Increase in calculation speed was approx. 250x.

19. Accurate and fast simulations of blasts impact on structures.

Another way of increasing simulation speed is through model reduction. An example is given on the development of a substitute structural element for a joint in an offshore platform. The required level of detail to represent the dynamic response of the joint up to failure was examined. For the conventional technique, either the cpu time (1.2 CPU year for the fine mesh) or the accuracy (1 CPU day for the coarse mesh) were unacceptable. Therefore the substitute element was developed, evaluated and implemented into the commercial LS-DYNA code. Accurate blast wall response predictions are obtained within $\frac{1}{4}$ CPU day. The result is that it becomes feasible to optimize such structures for weight and performance based on accurate analyses where currently over-conservative semi-empirical engineering

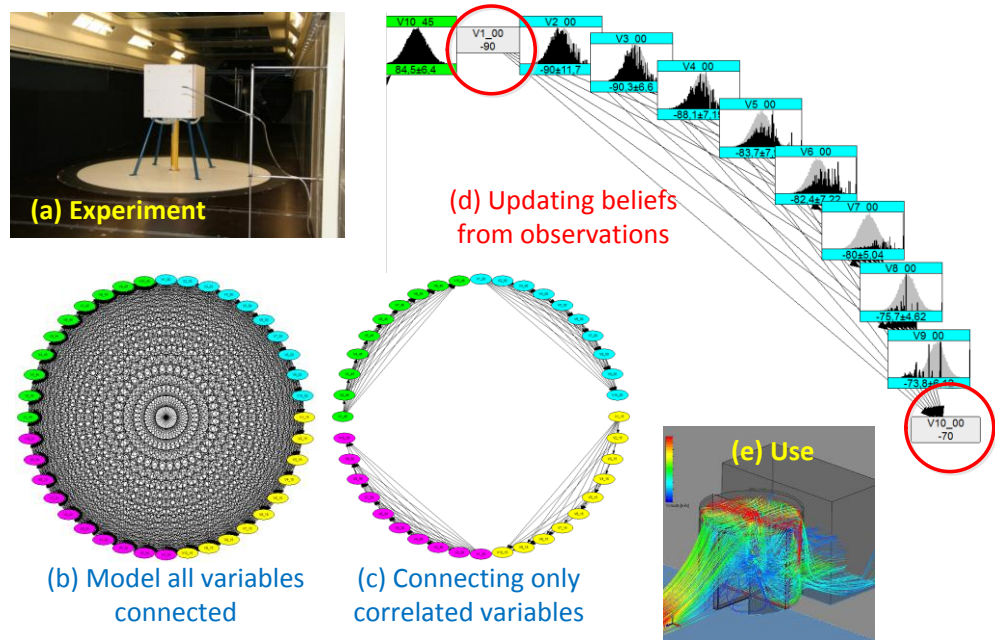
rules are used. This technique can also be used for analyzing crash/collision response of structures. A similar technique has been developed for predicting the response of brittle failure of fiber reinforced composite structures.



20. Update your beliefs in order to simplify empirical models and reduce uncertainty

We have worked on analysing wind tunnel experimental measurements (see Figure below). These data are often used to extrapolate the data to environmental conditions in buildings which in turn serve to advise authorities and particularly with respect to the reliability of the building. With a technique called Bayesian Networks we represent the variables of interest (that is the phenomena we want to model) as probability distributions (a frequency histogram for example) and the dependence between these as arrows going from one variable to another if such dependence exist (Figure, below panel a).

One feature for which BNs have contributed is to describe the dependence structure of the variables involved in the model. For example one may think that all variables depend on each other (Figure b). This hypothesis may be tested statistically and if two variables are found to be independent then the arc will be removed. The correct dependence model is simpler (Figure c) and facilitates not only the visualization of the model but also the calculus of probabilities. The simplified model may be used to “learn” on the basis of observations and update our uncertainty (reducing it). For example in Figure d observations on variables V1_00 and V10_00 become available, the updated uncertainty on the rest of the variables is shown in black while the original uncertainty (without observations) is observed in grey. In variable V8_00 the reduction of uncertainty is evident since the black histogram is more concentrated in the middle than the grey one. The updated beliefs may be used further for the quantification of physical models for industrial applications where Fluid Dynamics are involved or for the investigation of reliability of buildings with respect to wind loads (see Figure e).



Wind loads data may be obtained from experiments. These will be used to quantify probabilistic models also in terms of the correct representation of dependence. Later it will be used to update our beliefs on the basis of observations for example for reliability of buildings against extreme wind loads.

Together with our partners (TU Delft, Lighttwist Software) we have been able to quantify BNs with hundreds of variables. And make it possible to perform operations to the required accuracy in just seconds. That is, we are able to update our beliefs on certain variables after observing other variables in real time. This task was unthinkable even in the previous century without the use of very large and powerful computers. This opens the door to applications for example in monitoring where large amounts of data are obtained from sensors.

4 Signature

Utrecht, 15 April 2013

A handwritten signature in blue ink, consisting of several overlapping loops and strokes, likely representing the initials 'E.W.' followed by a surname.

Dr. ir. E.W. Meijer

Program Manager