Energy and Green House Gas Mitigation Technologies

Japan Society for the Promotion of Science-Imperial College London-University of Tokyo Symposium on Climate Change

Thursday 28th and Friday 29th September 2006

Imperial College London, South Kensington Campus, London SW7 2AZ

Imperial College London

energy futures lab

Simulation Technologies for New Energy Processes

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Imperial College
London

Providing plentiful and secure future energy supplies for both developed and developing countries, while addressing the environmental impact of energy production and use, is one of the key challenges facing our time.

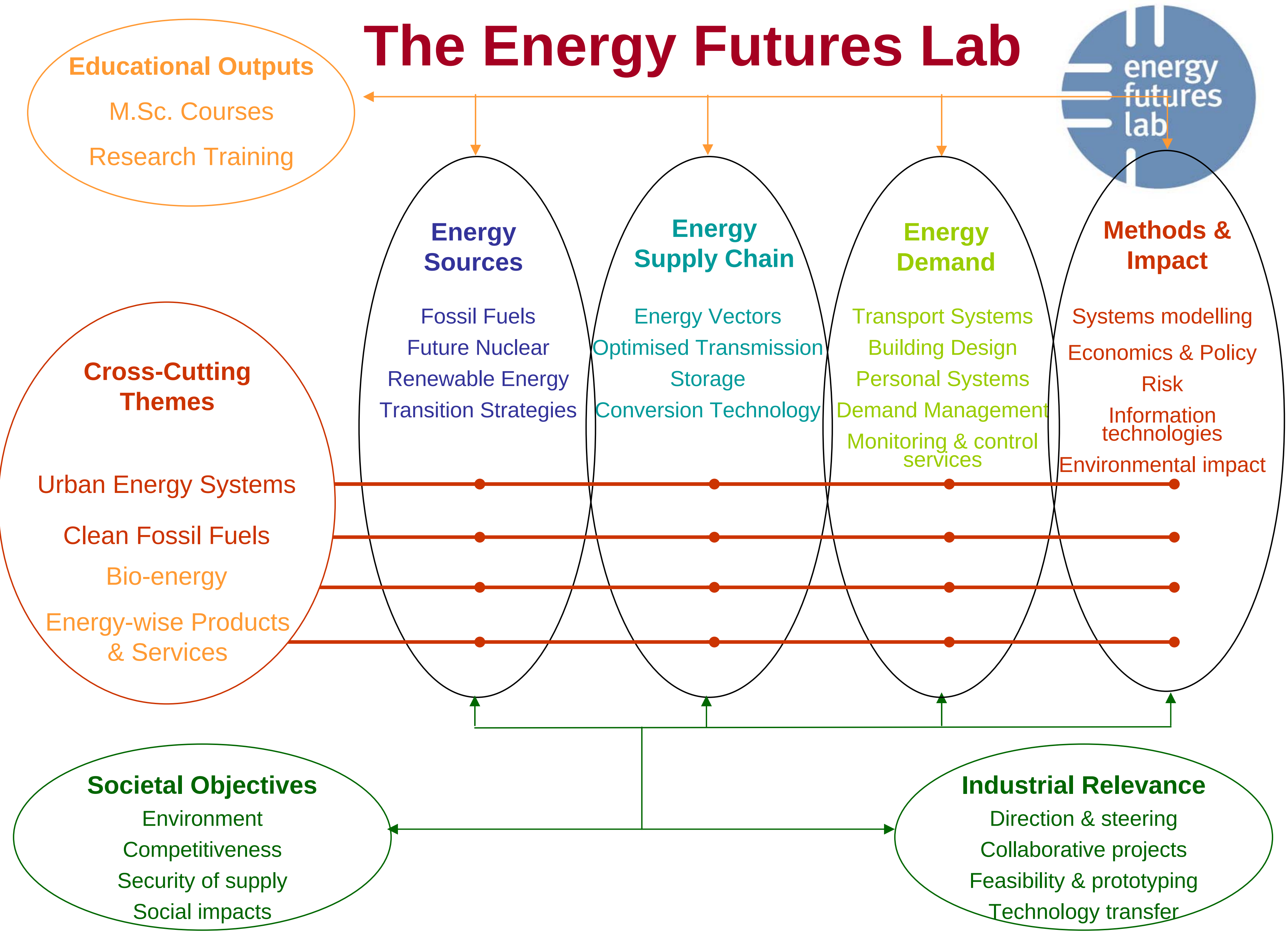
The **Energy Futures Lab** at Imperial College London is a major strategic research initiative which aims to play a leading role in setting the energy agenda over the next 20 to 50 years. It will focus the extensive energy portfolio of one the world's top research institutions on key issues, drawing on Imperial's wealth of knowledge in energy technologies and integrated systems design coupled with its proven track record in innovation and entrepreneurship.

Imperial College London tackles energy as one of its three strategic research priorities

Energy Futures Lab

Energy Futures Lab

Launched
2 November 2005


The Energy Futures Lab
energy futures lab
Educational Outputs
M.Sc. Courses
Research Training
Energy Sources
Fossil Fuels
Future Nuclear
Renewable Energy
Transition Strategies
Energy Supply Chain
Energy Vectors
Optimised Transmission
Storage
Conversion Technology
Energy Demand
Transport Systems
Building Design
Personal Systems
Demand Management
Monitoring & control services
Methods & Impact
Systems modelling
Economics & Policy
Risk
Information technologies
Environmental impact
Cross-Cutting Themes
Urban Energy Systems
Clean Fossil Fuels
Bio-energy
Energy-wise Products & Services
Societal Objectives
Environment
Competitiveness
Security of supply
Social impacts
Industrial Relevance
Direction & steering
Collaborative projects
Feasibility & prototyping
Technology transfer

Key points

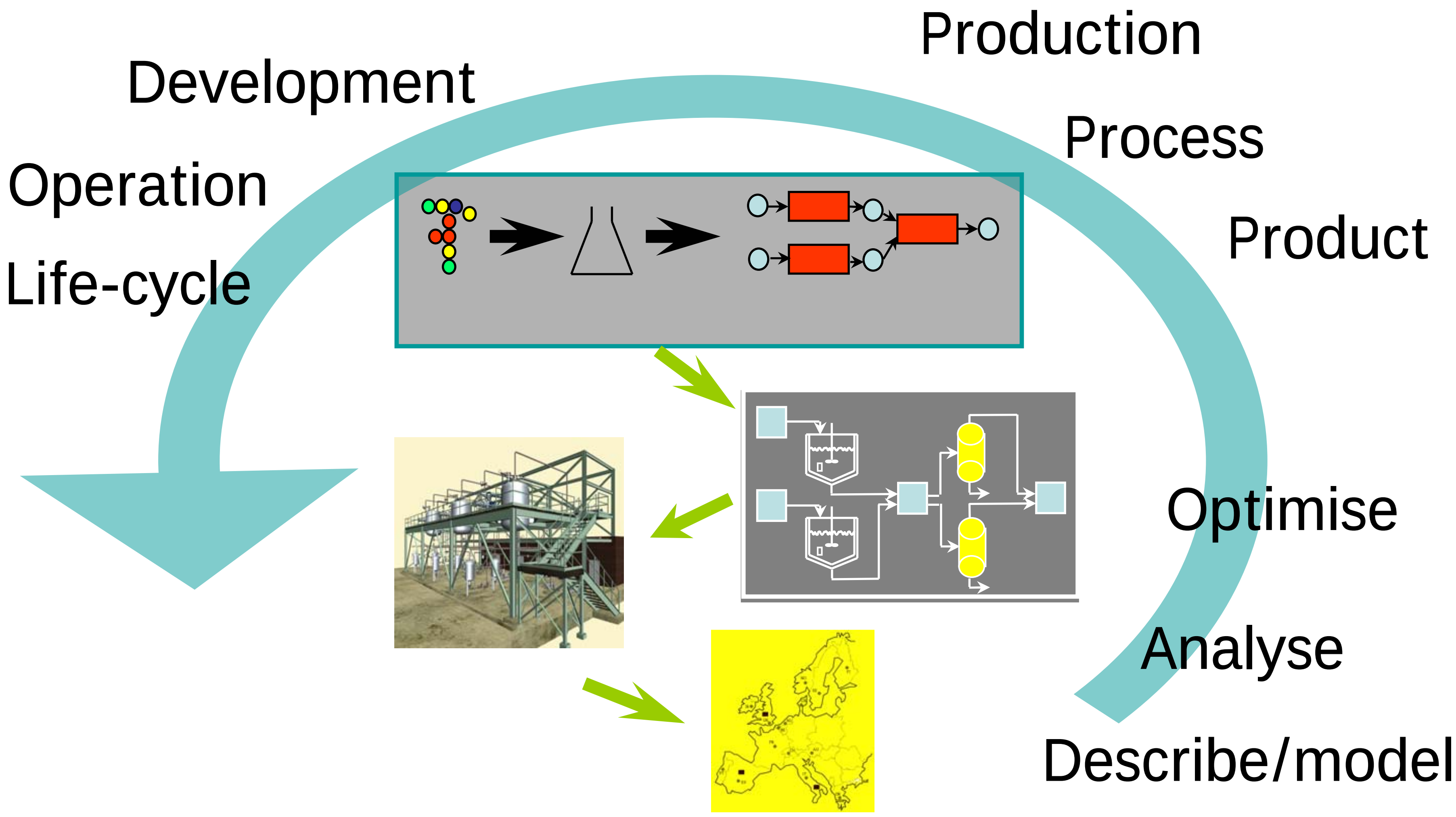
- simulation a key enabler of the first energy revolution (e.g. distillation, oil refining)
  - complexity, interactions, systems view

- a key enabler of current energy revolution
  - complexity, interactions, systems view

- new simulation technologies
  - Increase efficiency of current processes plenty of scope !
  - New technologies, products, processes even more so !

- some examples

Scope of “simulation”



Simulation & Energy

- 1950's LP, tray-by-tray distillation calculations, …
- 60'-70' Industrial simulators (Chiba, Esso, Monsanto, BP…)

First energy crisis - cannot do coal, solids, … !!

- 80's Specialisation (SimSci, Aspen, Hysis, Chemshare,…)
- 90's Consolidation (little innovation, 70's architecture)

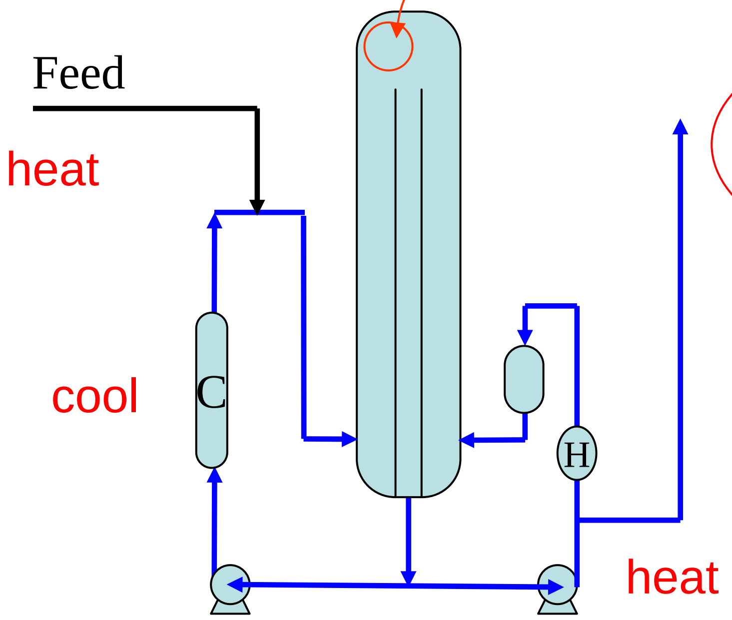
- 00's Emergency of dynamics, Sophisticated modelling /solution environments, distributed architecture, new capabilities
  ➔ e.g. gPROMS (Process Systems Enterprise)

New energy systems - far greater complexity, across multiple scales

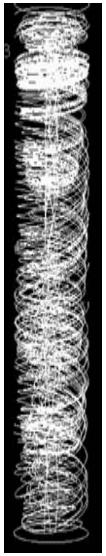
Multiscale example

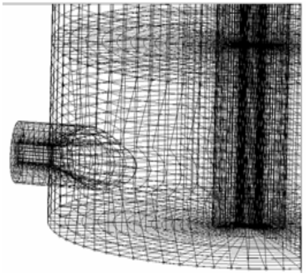
Crystallisation (energy intensive)

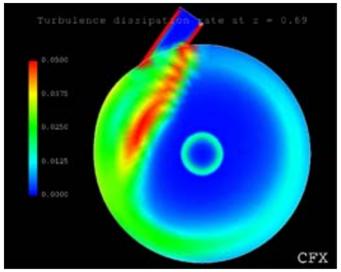
Detailed, local crystallization model ~4000 eq. !!



Mixing, Flow fields ~50.000 cells





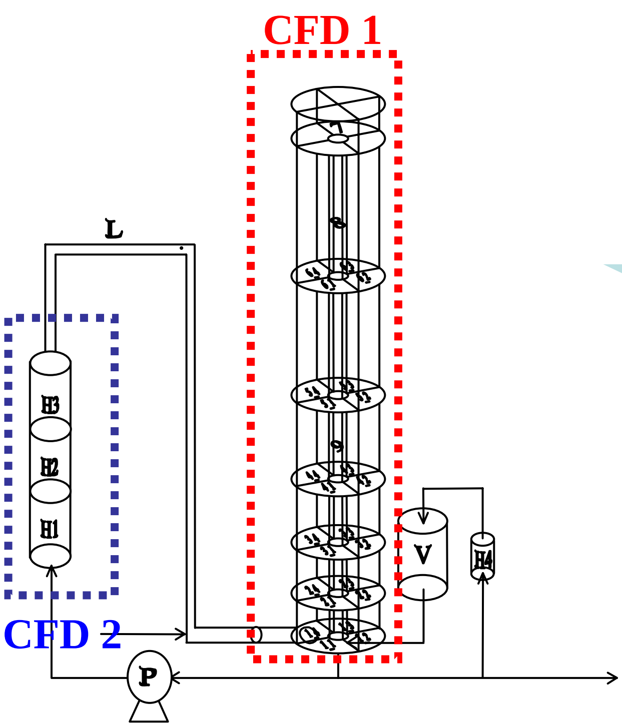


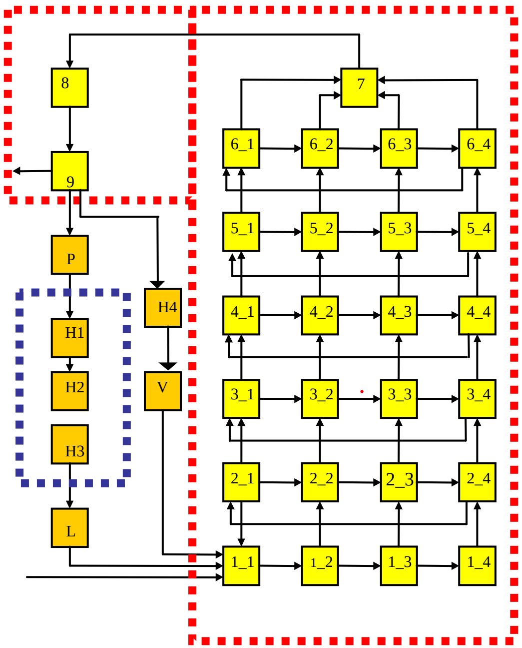
Courtesy of Mitsubishi Chemical Company

Simultaneous solution

CFD Model (Fluent)

gPROMS Model (PSE Ltd)



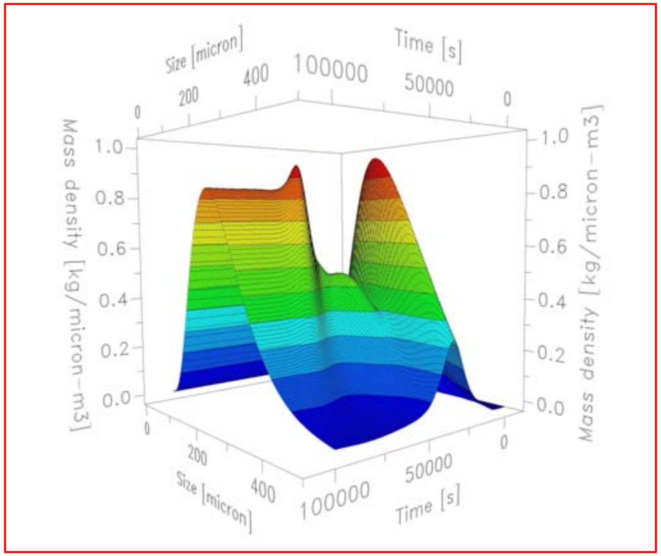


Courtesy of Mitsubishi Chemical Company

Crystal size distribution

- Accurate prediction of crystal size distributions
- Validated on full scale industrial plant
- Much improved operation, design

60% less energy !



Incorporate geometry

Scale-up / Scale-down

General way to model

and solve multiscale

CFD + simulation problems

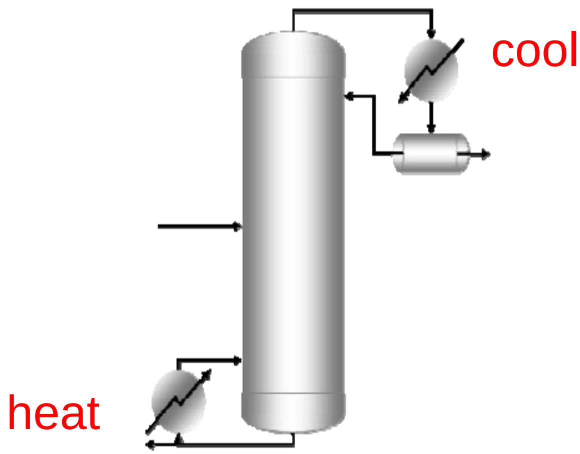
Courtesy of Mitsubishi Chemical Company

Distillation

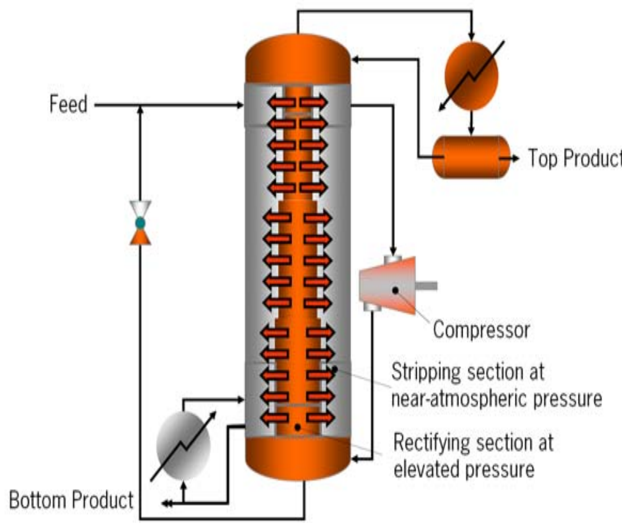
very old (sake, whisky, …),   pervasive

extensively optimised

~40% of energy used by Chemical Process Industries



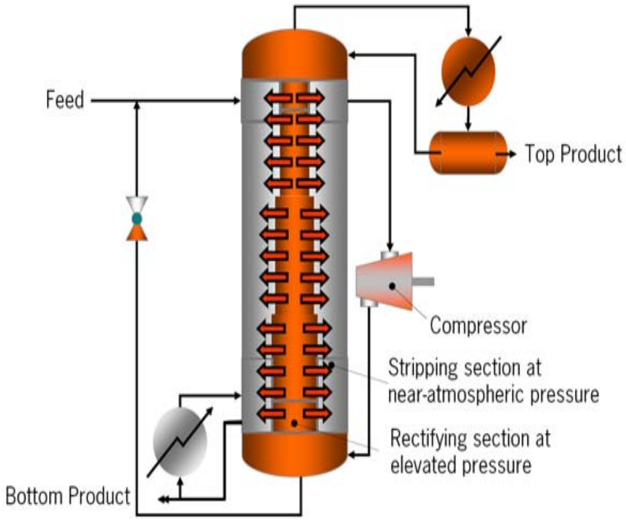
Traditional

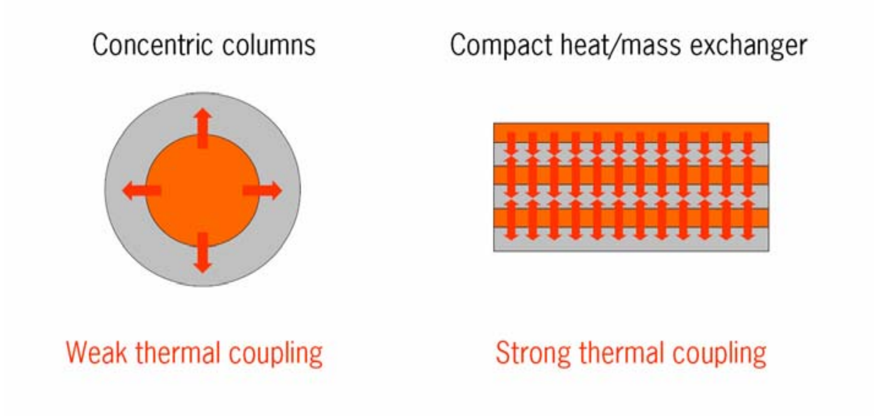


Heat Integrated

Courtesy of Process Systems Enterprise Ltd

Heat Integrated Distillation Columns - HIDiC





BTX case study:

Heat Integrated — 56% of conventional column heating / cooling + compact !

BUT difficult to start-up & control; very narrow operating window

detailed model, dynamic analysis & control optimisation ➔ great performance !

Ongoing HIDiC project

2006-2007 (2 years)

AIST
•Organizer of this project
GL: Dr. Nakaiwa

Maruzen Petrochemical Co., Ltd.
•R&D of HIDiC operatability

Kansai Chemical Engineering Co., Ltd.
•R&D of tray column type HIDiCs

Kimura Chemical Plant Co., Ltd.
•R&D of shell & tube, packed column and wetted wall types HIDiCs

Mitsubishi Chemical Corporation
•Development of simulation technology

Toyo Engineering Corporation
•Development of Engineering technology

Kyoto University
•Process synthesis technology

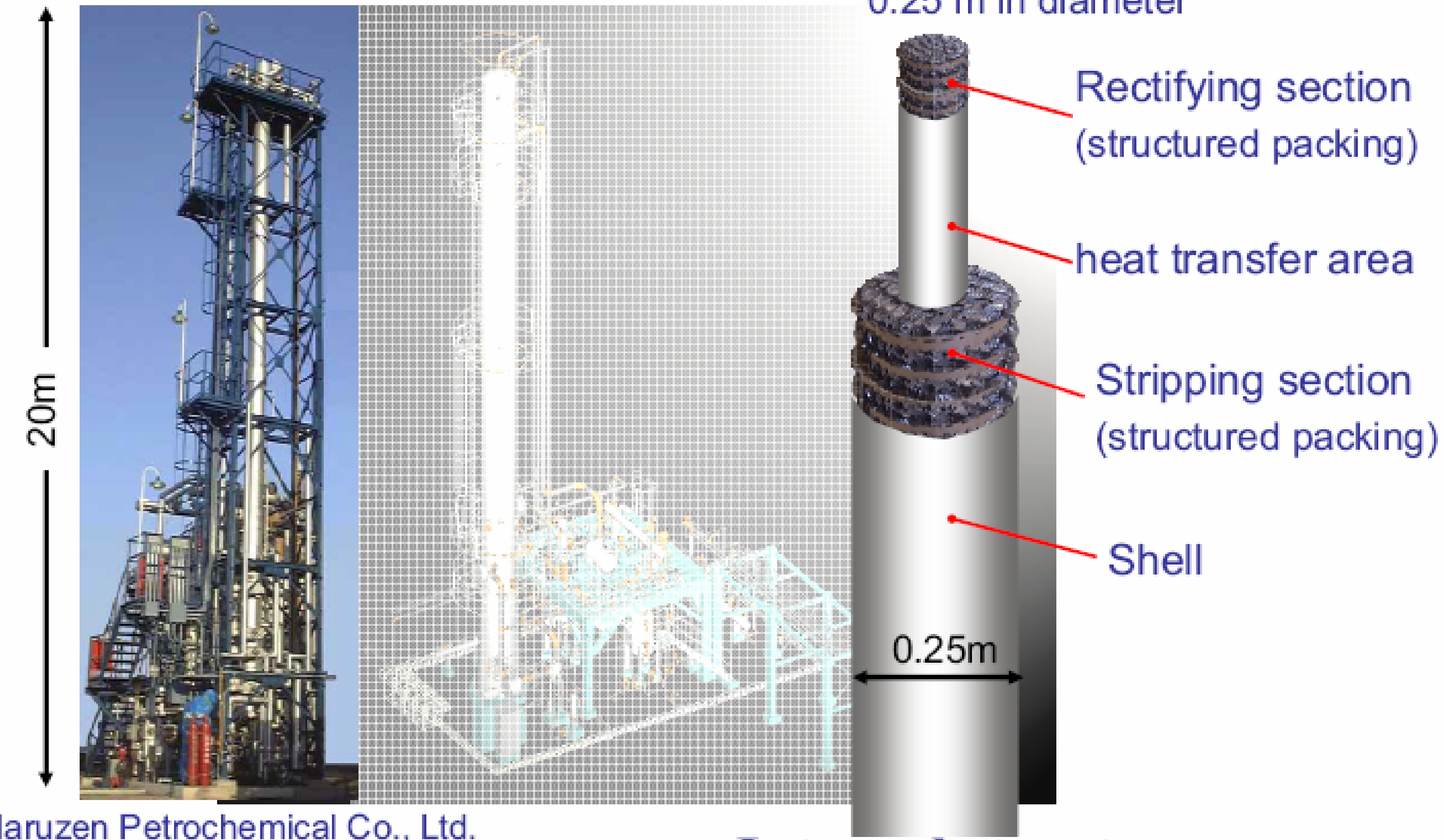
Nagoya Institute of Technology
•Control technology for safe operation

Tokyo Institute of Technology
•Heat and mass transfer

The Bench Plant of HIDiC in Japan

The bench plant was built in 1999.

16 m in height
0.25 m in diameter



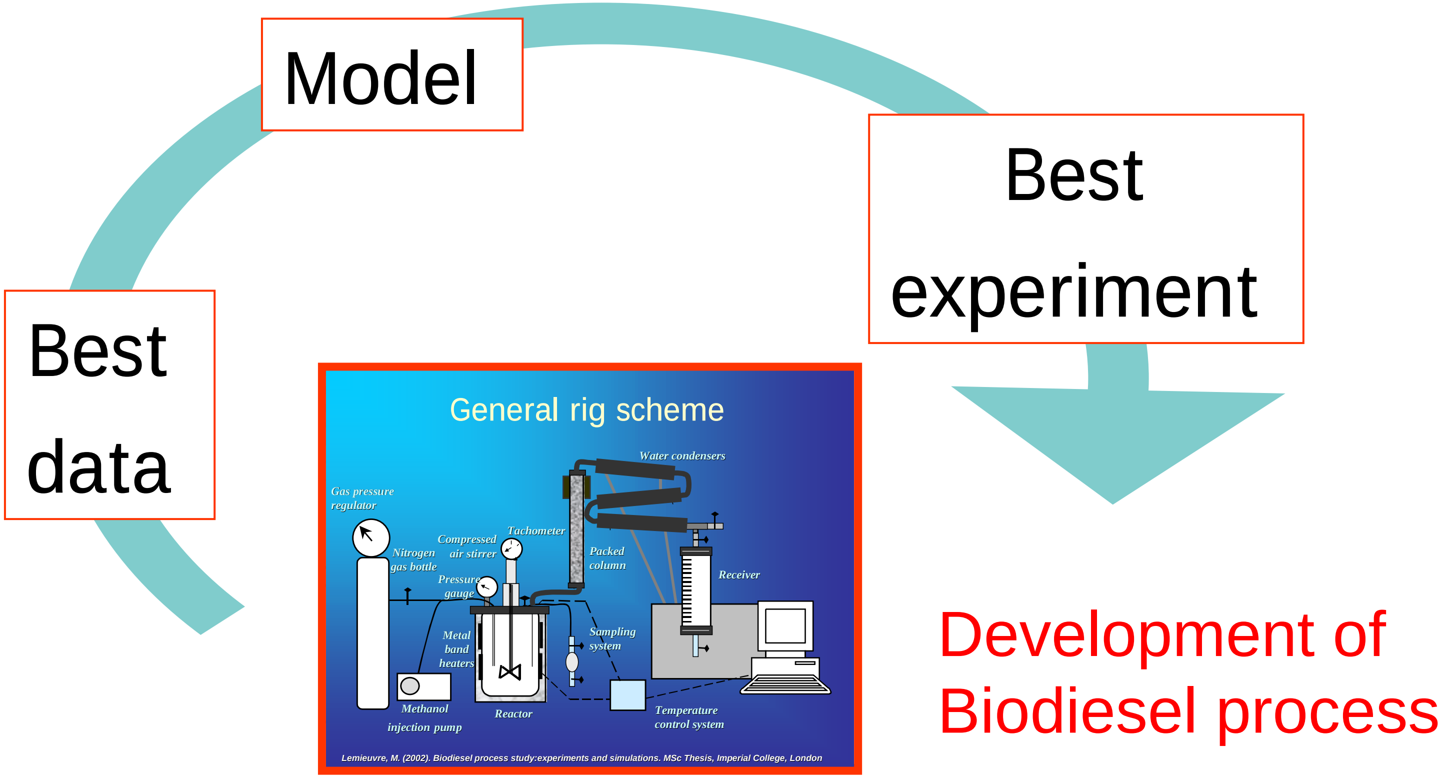
Maruzen Petrochemical Co., Ltd.
Kimura Chemical Plants Co., Ltd.

Internal structure

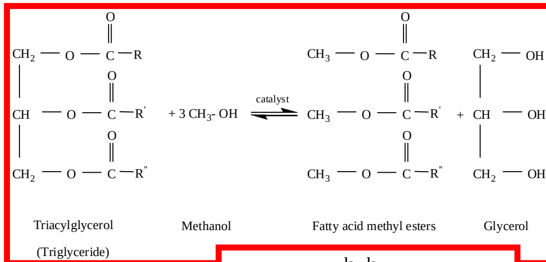
Courtesy of Process Systems Enterprise

Model validation

- Model + Data ➔ parameters
- Statistics – Lack of fit, confidence regions, …
- Model-based Design of Experiments



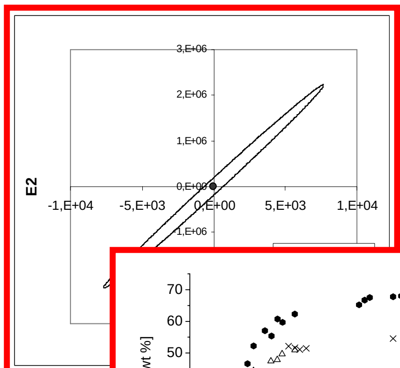
Biodiesel process development

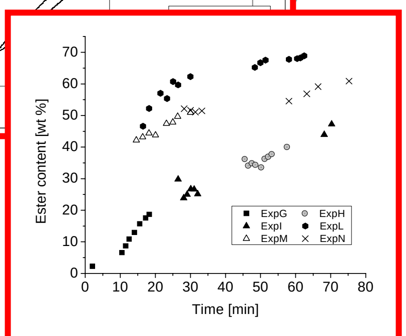


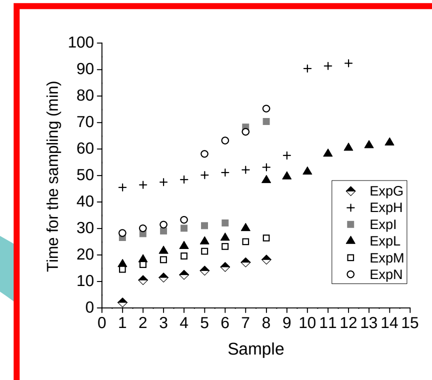
$$TG + M \underset{}{\overset{k_1,k_2}{\longleftrightarrow}} DG + E$$

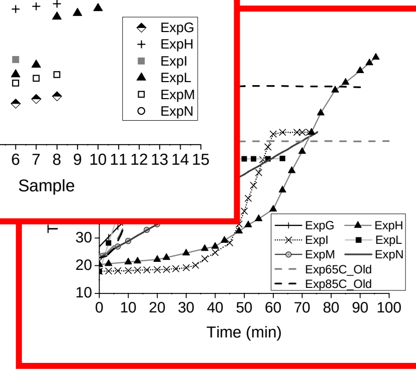
$$DG + M \underset{}{\overset{k_3,k_4}{\longleftrightarrow}} MG + E$$

$$MG + M \underset{}{\overset{k_5,k_6}{\longleftrightarrow}} G + E$$





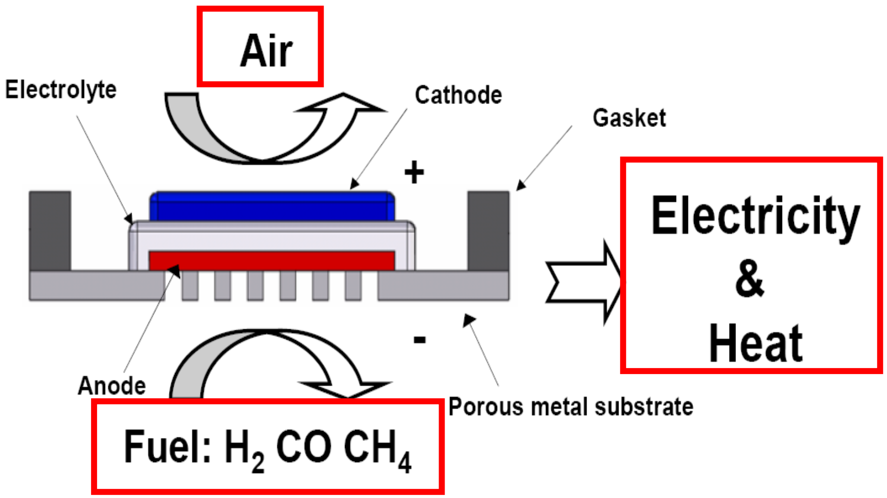


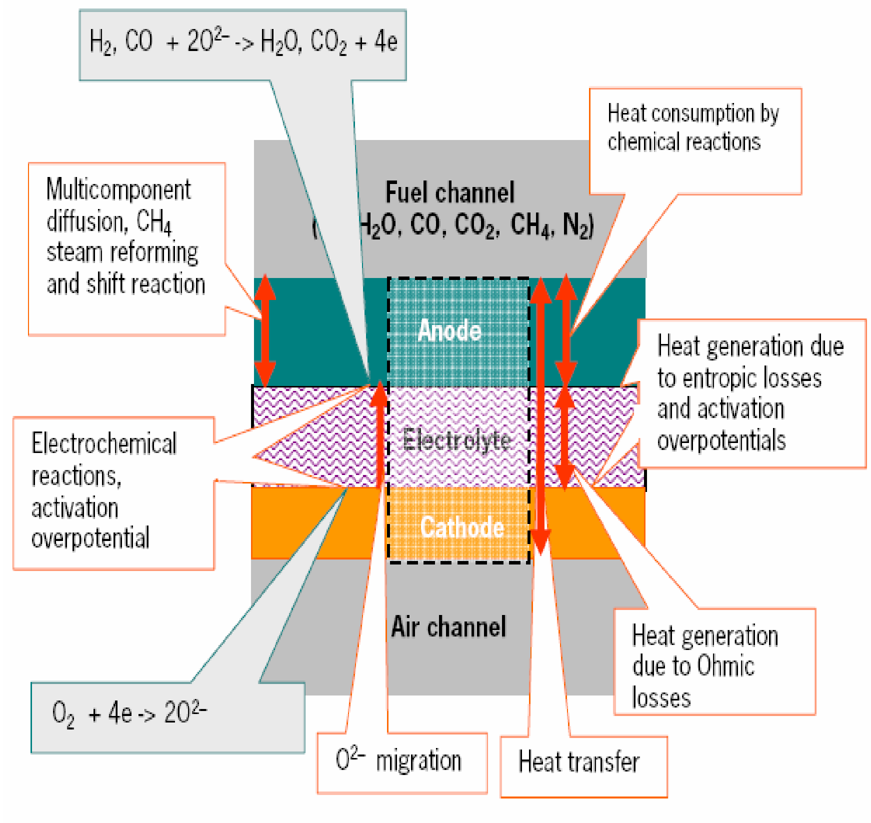


Substantial opportunities for simpler, cheaper better processes

Fuel cell

Solid Oxide Fuel Cell (SOFC) membrane

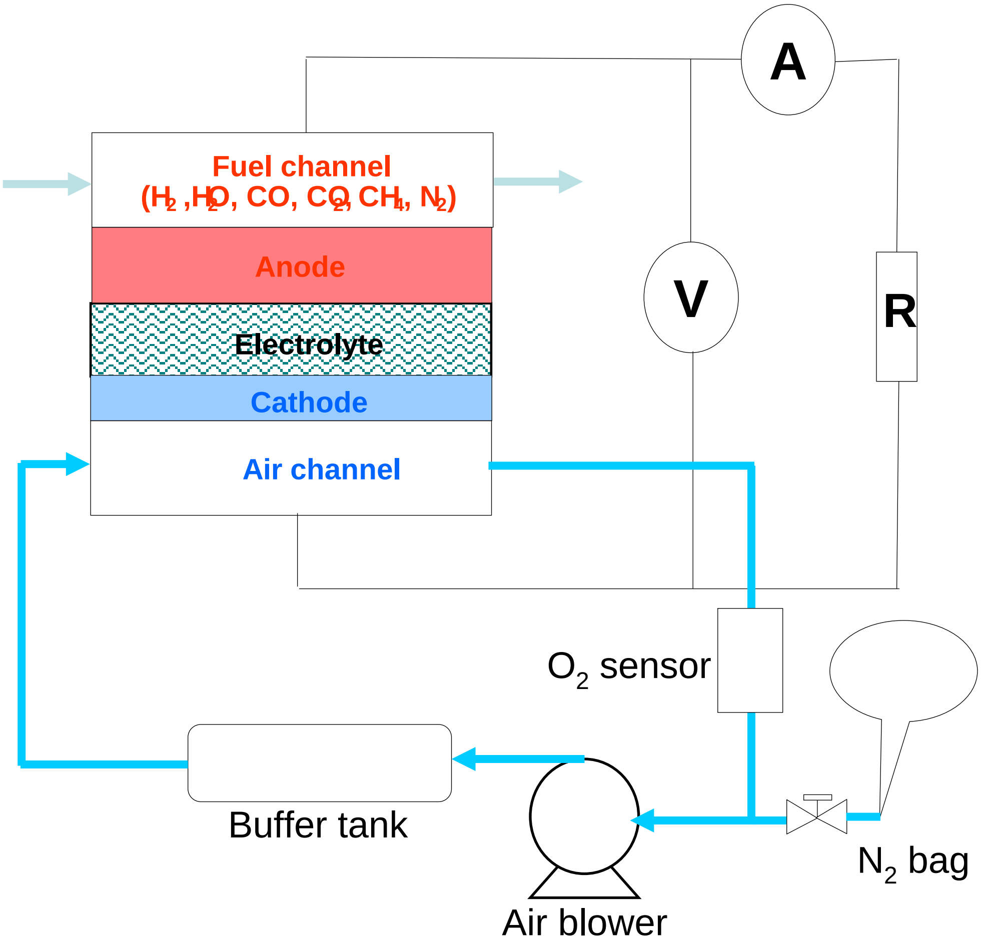




High fidelity models of physics, chemistry and electrochemistry

Courtesy of Process Systems Enterprise Ltd

Model validation : Closed-loop experiment

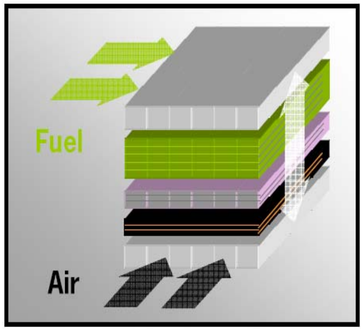


- A novel experimental technique – designed by PSE for use during FC development
- Valuable source of complementary data
- Ensures uniform conditions across the cell and allows full control of the fuel utilisation
- Sufficiently accurate to identify electronic leakage at low current densities
- The flow-through and closed loop data are processed simultaneously using gPROMS parameter estimation

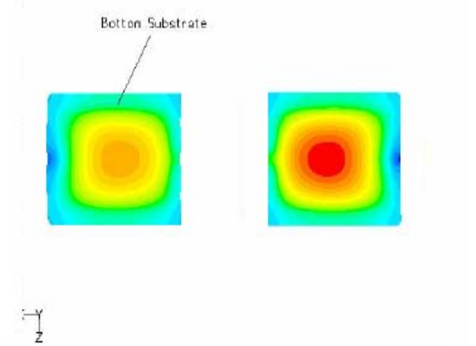
Fuel cell

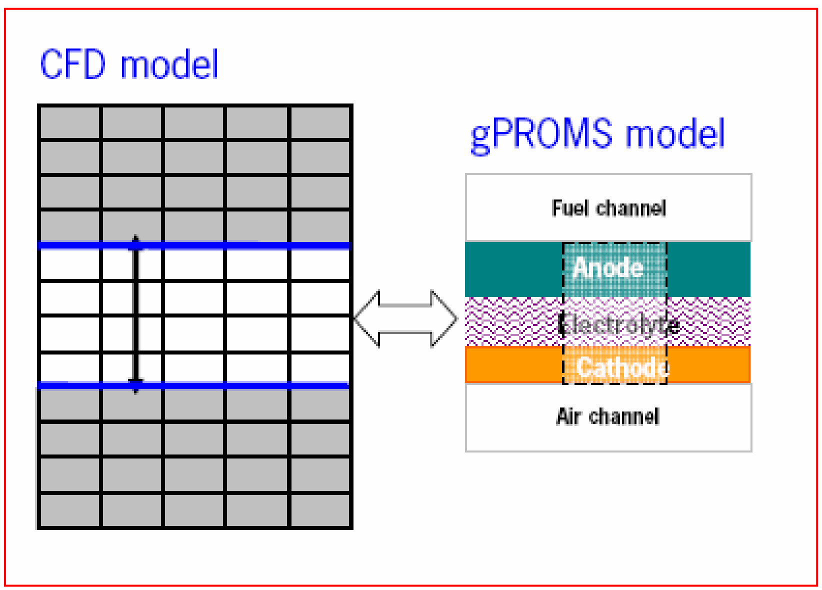
SOFC stack

- mass and heat transfer at gas-solid interfaces
- effect of air & gas geometry and flow distribution
- heat losses
- dynamic response

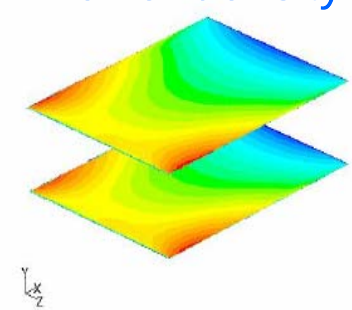


Temperature contours





Power density



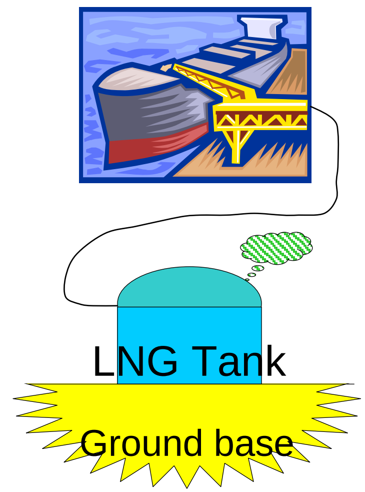
Combined solution allows analysis of complex channel geometries

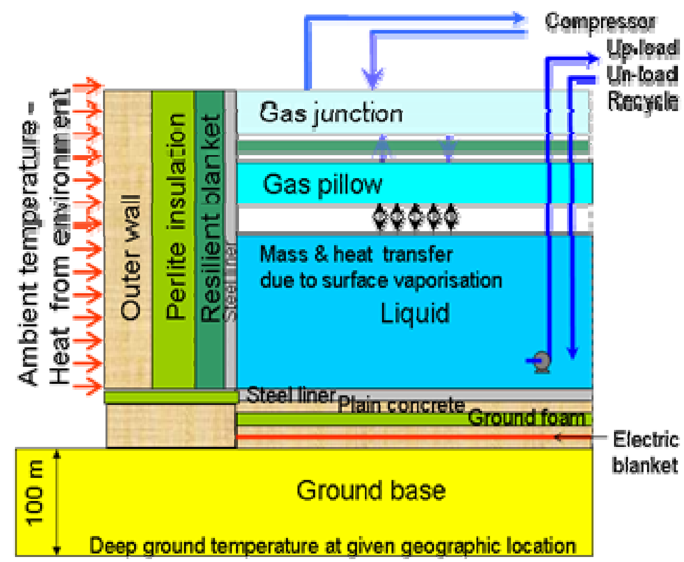
Fuel cells - a modular library

- An integrated strategy for FC modelling
  - I. solid membrane
  - II. experiments, data processing, model validation
  - II. fuel cell/stack
  - III. power plant
  - IV. electrical network
- …aiming to achieve
  - model consistency
  - model re-usability
- …across the FC development lifecycle
  - from model validation to control system design
- Generally applicable to all types of FC
  - SOFC, PEMFC, DMFC, …

Conventional steel-lined LNG storage tanks

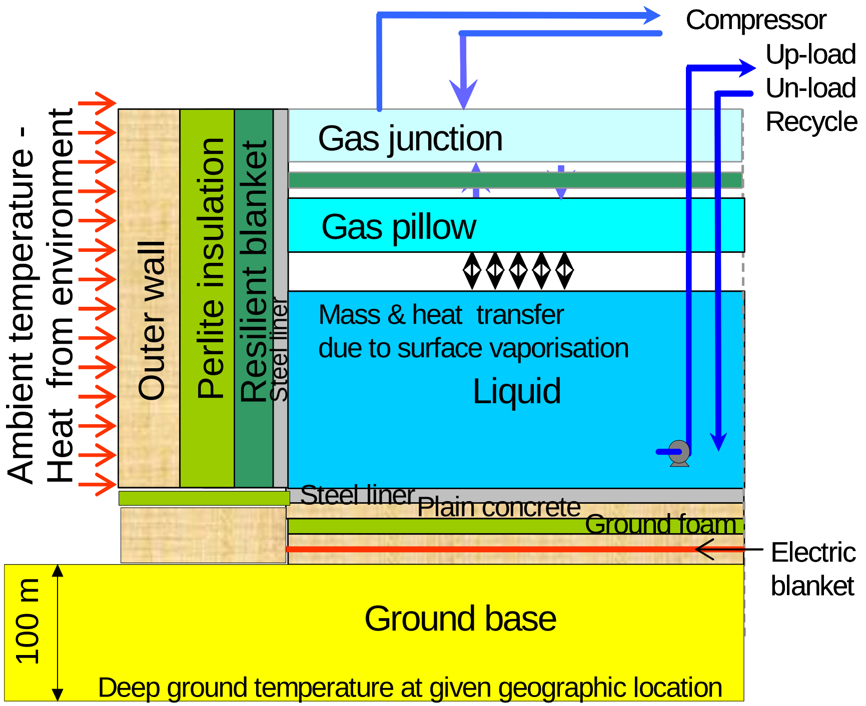
- Capital-intensive design decisions
  - scale of equipment
  - adverse operating conditions
- Operation is transient
  - difficult to "guess" the optimal solution (or even a feasible one)
- Underlying physics relatively well understood
  - models can be fully predictive
  - there is no need (and little scope) for experiments
- Modelling can provide important support to design decisions
  - sometimes a single YES/NO question needs to be answered
  - potential financial impact very significant





Modelling objectives

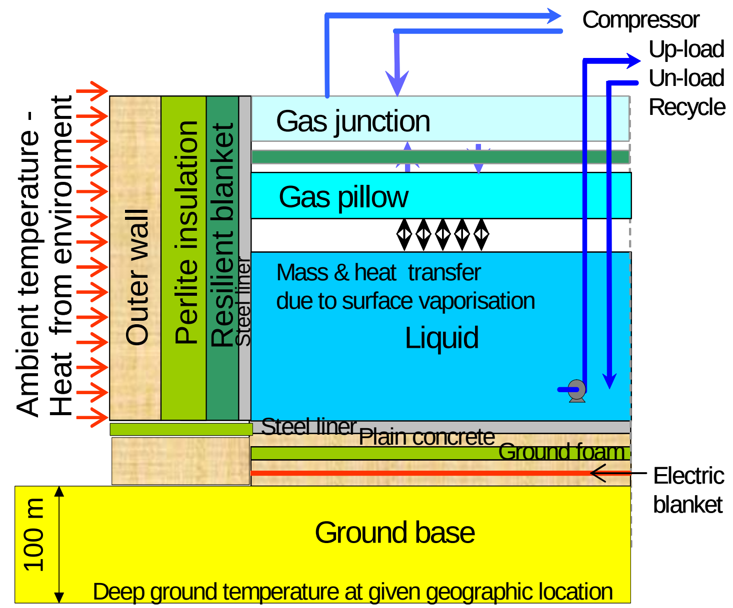
- Predict
  – heat gain from environment
  – dynamics of tank “breathing”



- so as to optimise…
  – amount of insulation
  – power supply to electric blanket

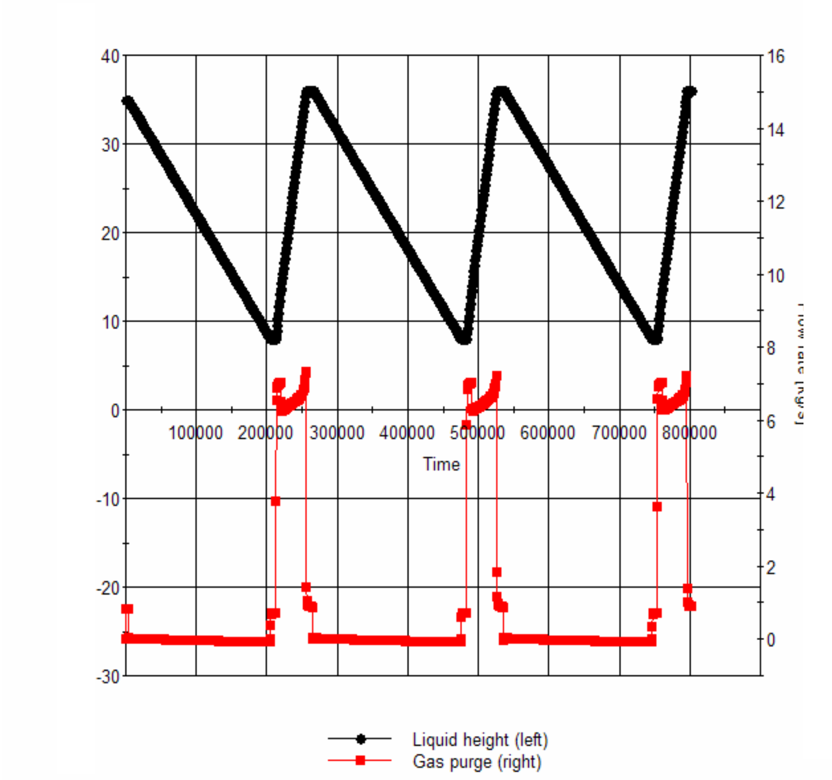
The gPROMS LNG storage tank model

- Mass & energy balances of the liquid in tank
- Rigorous dynamic 2d model of heat conduction in
  - all component layers
  - the ground base
- Moving liquid surface
  - due to loading, unloading, evaporation
  - affects heat transfer characteristics
- Mass/heat transfer at the liquid surface

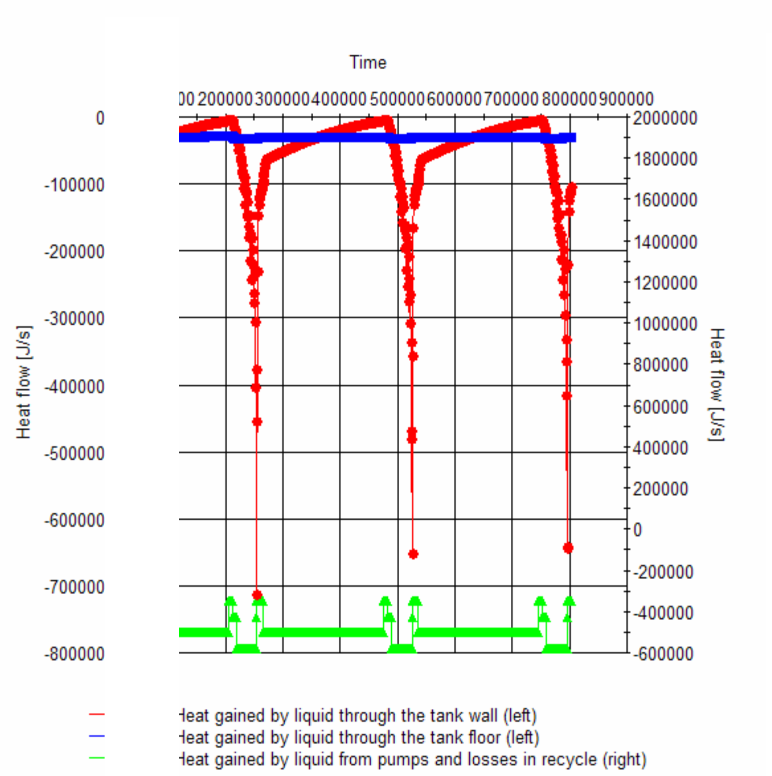


Selected results

Liquid height and gas purge over 3 cycles



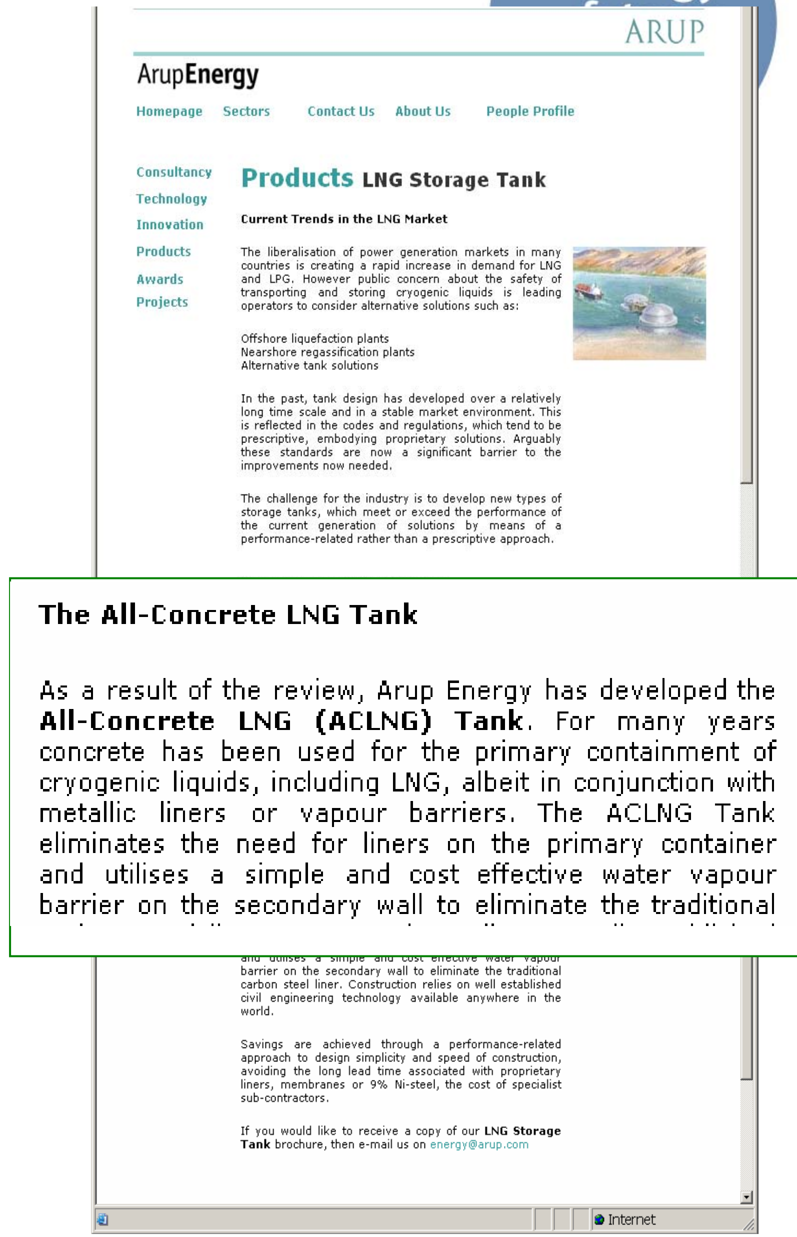
Heat gained by liquid



All-concrete LNG tanks (ACLNG)

- Do not include the steel lining
- Save
  - cost of steel
  - ~25% off construction schedule
- Not really a new idea: mentioned in academic papers from the 1980s
  - Imperial's Civil Engineering Department
- Renewed interest in the industry in the 2000s

- **Key issue: management of risk associated with LNG permeation through concrete**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Products **LNG Storage Tank**

Current Trends in the LNG Market

The liberalisation of power generation markets in many countries is creating a rapid increase in demand for LNG and LPG. However public concern about the safety of transporting and storing cryogenic liquids is leading operators to consider alternative solutions such as:

Offshore liquefaction plants
Nearshore regassification plants
Alternative tank solutions

In the past, tank design has developed over a relatively long time scale and in a stable market environment. This is reflected in the codes and regulations, which tend to be prescriptive, embodying proprietary solutions. Arguably these standards are now a significant barrier to the improvements now needed.

The challenge for the industry is to develop new types of storage tanks, which meet or exceed the performance of the current generation of solutions by means of a performance-related rather than a prescriptive approach.

The All-Concrete LNG Tank

As a result of the review, Arup Energy has developed the **All-Concrete LNG (ACLNG) Tank**. For many years concrete has been used for the primary containment of cryogenic liquids, including LNG, albeit in conjunction with metallic liners or vapour barriers. The ACLNG Tank eliminates the need for liners on the primary container and utilises a simple and cost effective water vapour barrier on the secondary wall to eliminate the traditional carbon steel liner. Construction relies on well established civil engineering technology available anywhere in the world.

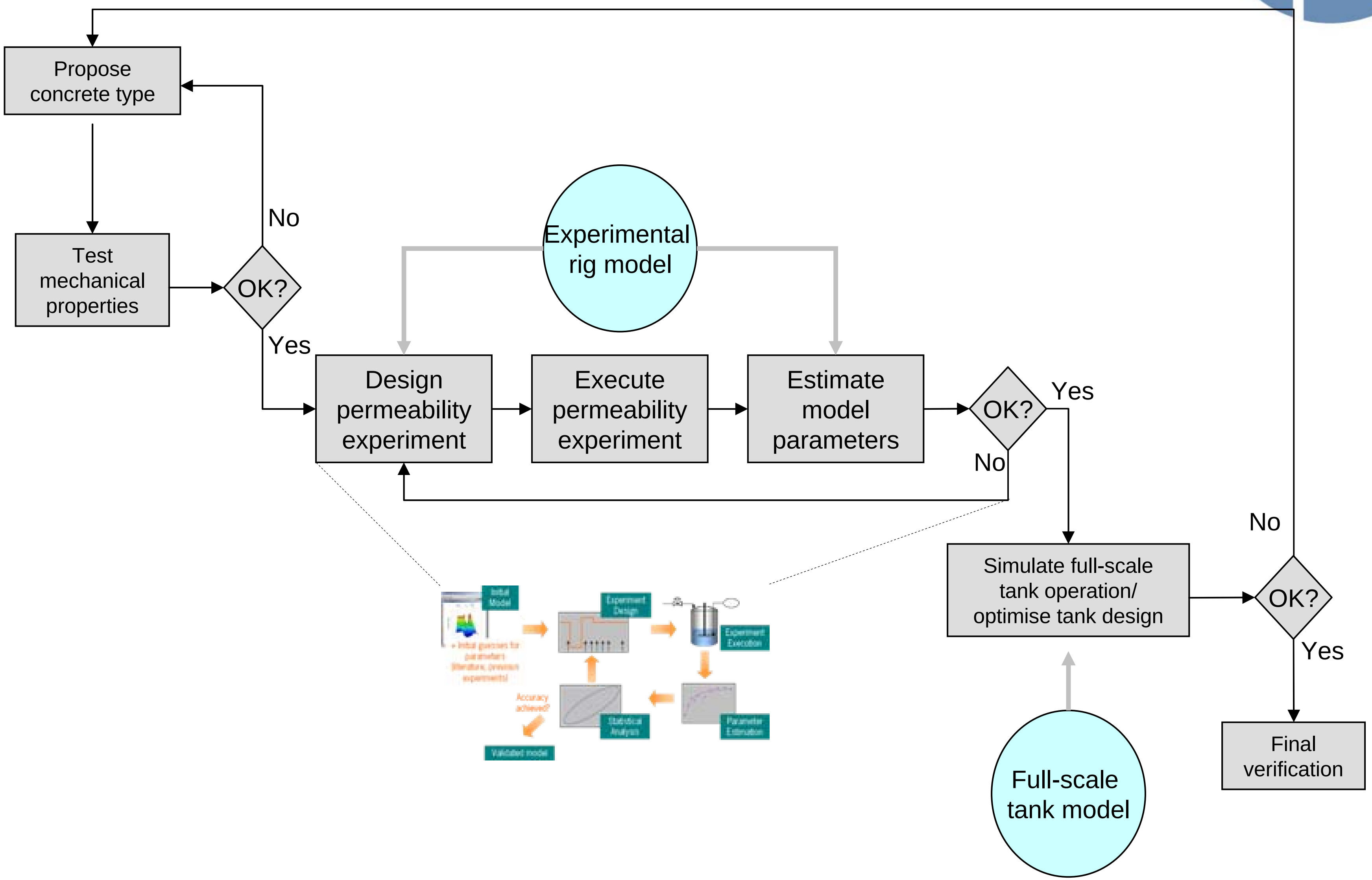
Savings are achieved through a performance-related approach to design simplicity and speed of construction, avoiding the long lead time associated with proprietary liners, membranes or 9% Ni-steel, the cost of specialist sub-contractors.

If you would like to receive a copy of our **LNG Storage Tank** brochure, then e-mail us on energy@arup.com

Internet

Design of all-concrete LNG tanks

Integrated experimental/modelling procedure



In summary

- Most energy applications involve complexity, interactions, trade-offs, risk ➔ a whole system approach
- Modelling-Simulation-Optimisation is a key enabler
- A new generation of methods and software can handle vastly increased complexity, with ease of deployment
  - High fidelity, Nonlinearities, Interactions, Validation, Multiscale, Dynamics, Optimisation, …
- Many successful applications on a wide range of energy problems:
  - Dramatic improvements of “traditional” energy-hungry designs, operations
  - Development of radically new concepts, equipment, process designs
  - Detailed analysis often reveals and exploits counter-intuitive solutions

Lean & green

energy futures lab

Thanks for your attention

www.imperial.ac.uk/energyfutureslab

Energy efficiency - a primary source ?

Transport : ~ 50% of oil

Average fleet economy, cars & light trucks (mpg)

	2004	planned/approved
EU	37	44 (2008)
Japan	45	48 (2010)
Canada	25	32 (2010) proposal
China	29	37 (2008)
USA	24	no target
California	?	36 (2015)
2004 Toyota Prius	55	

US fleet as efficient as EU TODAY	~3 MBD
Kazakhstan output in 5-10 yrs	~2 MBD ➔ 4MBD
US imports from Gulf	~2.7MBD
BP entire production	~4 MBD

Transport : where does half the world oil go?

Oil →	petrol →	wheel turning →	mass moving
100	94	12.2	0.6 passenger
			11.6 car

heat, noise !

1/3 aerodynamic drag
1/3 rolling resistance
1/3 acceleration/brakes

Volkswagen Golf – over 30 years

x 1.5 fuel efficiency
x 2 weight

1 unit of “person transport” energy = 100/0.6 = 166 units of oil energy