STEP BY STEP

ACHIEVING RAPID RESULTS WITH AN INCREMENTAL APPROACH TO MODEL DEVELOPMENT

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Performance you can rely on.

Infineum

An introduction to Infineum

- Infineum is a world leader in the formulation, manufacturing and marketing of petroleum additives for lubricants and fuels
- Established in 1999 as a joint venture between ExxonMobil and Shell
- Innovative products for
  - Automotive, heavy duty diesel and marine engine oils
  - Diesel fuels
  - Speciality applications such as transmission fluids and industrial oils
- Manufacturing Technology are the stewards of product quality
- Infineum have used gPROMS to model several processes

Additives in the engine

Soot and deposits cause abrasion and clogging

Hot metal parts grind against each other, causing wear

Additives prevent deposits from causing problems

Additives protect engines from mechanical wear and corrosive reactions

Temperatures range from below freezing to above boiling

Additives keep engines working smoothly at all temperatures

Additive chemistry

- Transport additive used in engine oils
- Two raw materials, A and B

$$A + B \rightarrow AB$$
$$AB + B \rightarrow AB_2$$

- We can measure conversion of A and conversion of B
- New grade with higher proportion of AB_2 and possibly including AB_3
  - What do we need to change to make this grade?
  - Adding each additional unit of B is much harder – reaction needs to be forced onwards

Building a simplified model

- Modelled a single-phase, well-mixed system

- A has several different isomers, only one of which is reactive
  - Added the isomer content of A
  - Allows model to accurately simulate A from any of our worldwide sources

- Started with just two isothermal reactions
  - Added AB_3 when the model couldn't match real conversions without it

$$AB_2 + B \rightarrow AB_3$$

  - Developed temperature-dependent Arrhenius equations for all reactions

- A can be isomerised when a catalyst, C, is added to the system

$$A_r \longleftrightarrow A_{ur} \quad \textit{in presence of C}$$

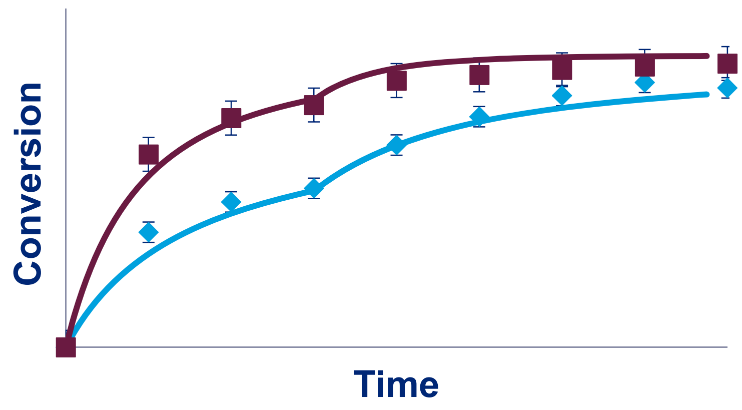
  - Added C into the model once the reactions of A and B were included and accurate

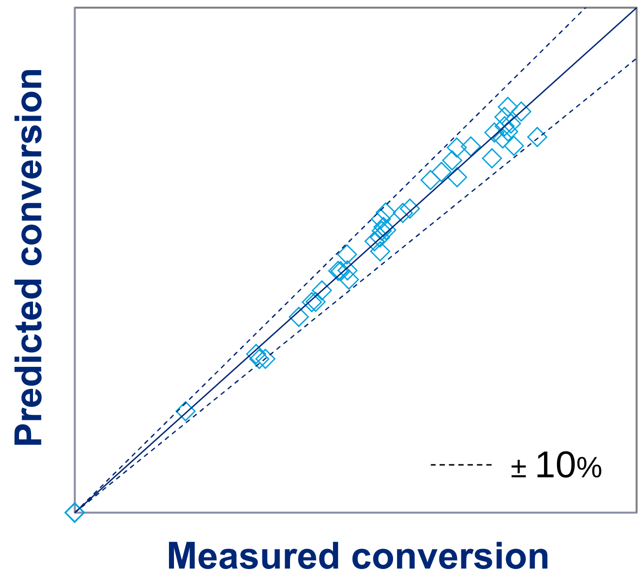
Efficient experimental work

- Close collaboration between experimental team and model developers
- Ran experimental program alongside model development
  - Feedback on which experiments and measurements were most useful
  - No redundant experiments
- Experimental plan designed specifically for modelling
  - Stepped away from the process we use on the plant
  - Experiments designed to show big changes
- Focus on gathering reliable quantitative data showing strong trends
- High quality data made parameter estimation accurate and easy

Getting a good fit

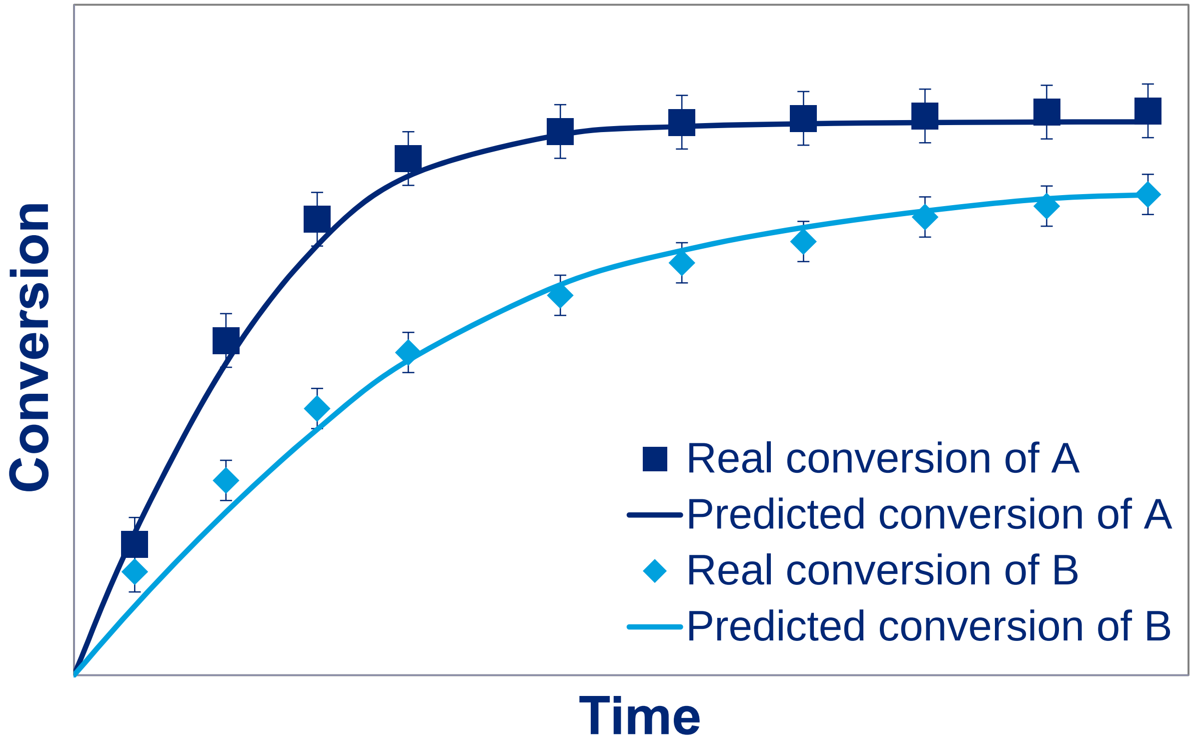
- Parameter estimation from lab data generated a good fit for the conversion data
- Model estimation of activation energy was within 1% of theoretical prediction
- Predicted results of new experiments to within ±10%



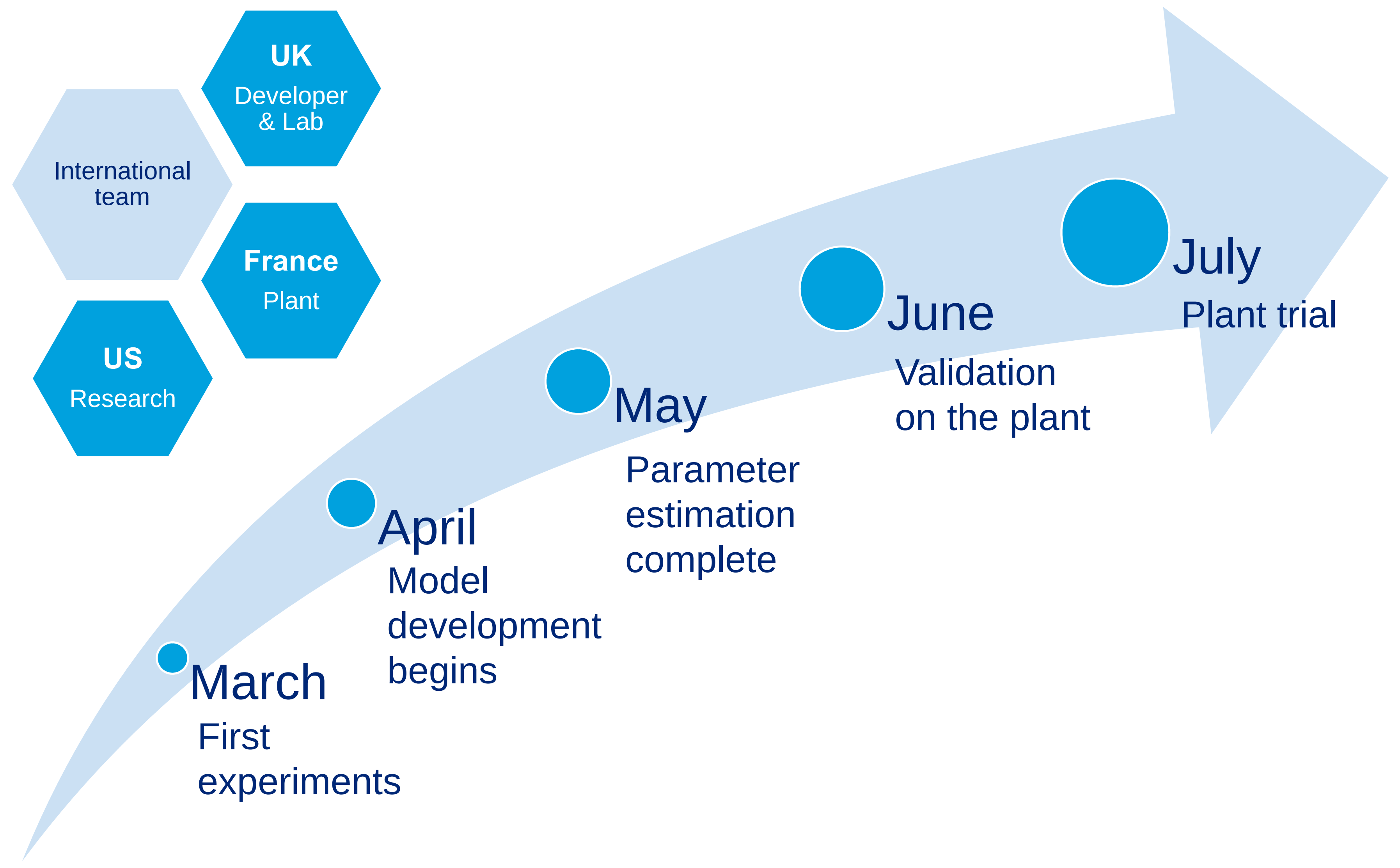


The real test: plant trials

- Carried out mini-trials changing one variable (temperature, charge of B, etc) at a time
- Model's good predictions gave plant confidence to run a trial with all variables changed at once



Team and timeline



Using the model: design of new reactors

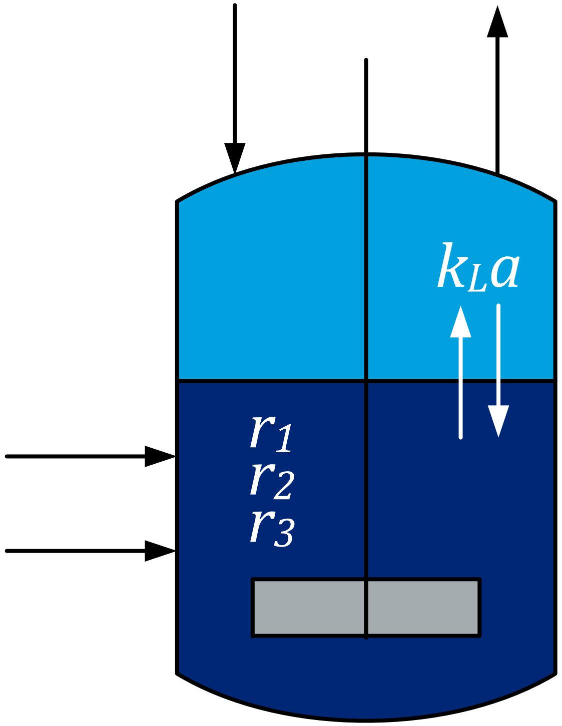
- New equipment will be built to manufacture our new additive grade
- Model allows us to calculate cycle times for many different production scenarios
- Also gives us the capability to explore continuous processing options
- Contrast to traditional approach to process design
  - No kinetic data
  - Design based on direct scale-up from lab or what we already have in other plants
  - Need to mitigate the risk of not knowing for sure if a new design will make the right product
- New tools such as modelling give us improved understanding and confidence for designing equipment

Using the model: on the plant

- Better understanding of when we reach the end point means we can run with more aggressive conditions
- Investigating integration of model into plant control systems, to give operator information about when batch is finished
- Potential 10% increase in capacity without any capital investment
- Plant can adapt to unexpected delays or conditions and still make on-spec products

Developing the model further

- Process involves some undesirable side reactions
- Modelling could help us pinpoint which mechanisms are dominant
- A working model which includes these side reactions would help us optimise our product
- Including these side reactions will probably require mass transfer and thermodynamics to be included in the model



Conclusions

- An accurate-enough model that works now can be more useful than a highly-accurate model that will work next year
- Development process is much faster when you start simple
- Only adding complexity when the data shows you need to reduces wasted effort and provides insights into key mechanisms and species
- Good model development relies upon a good experimental program
- An accurate model gives the plant confidence to make aggressive changes and reap big rewards