sasol
reaching new frontiers


# ***Holistic optimisation***
*An industrial case study*

better together...we deliver

# Sasol – a brief introduction

# Sasol snapshot

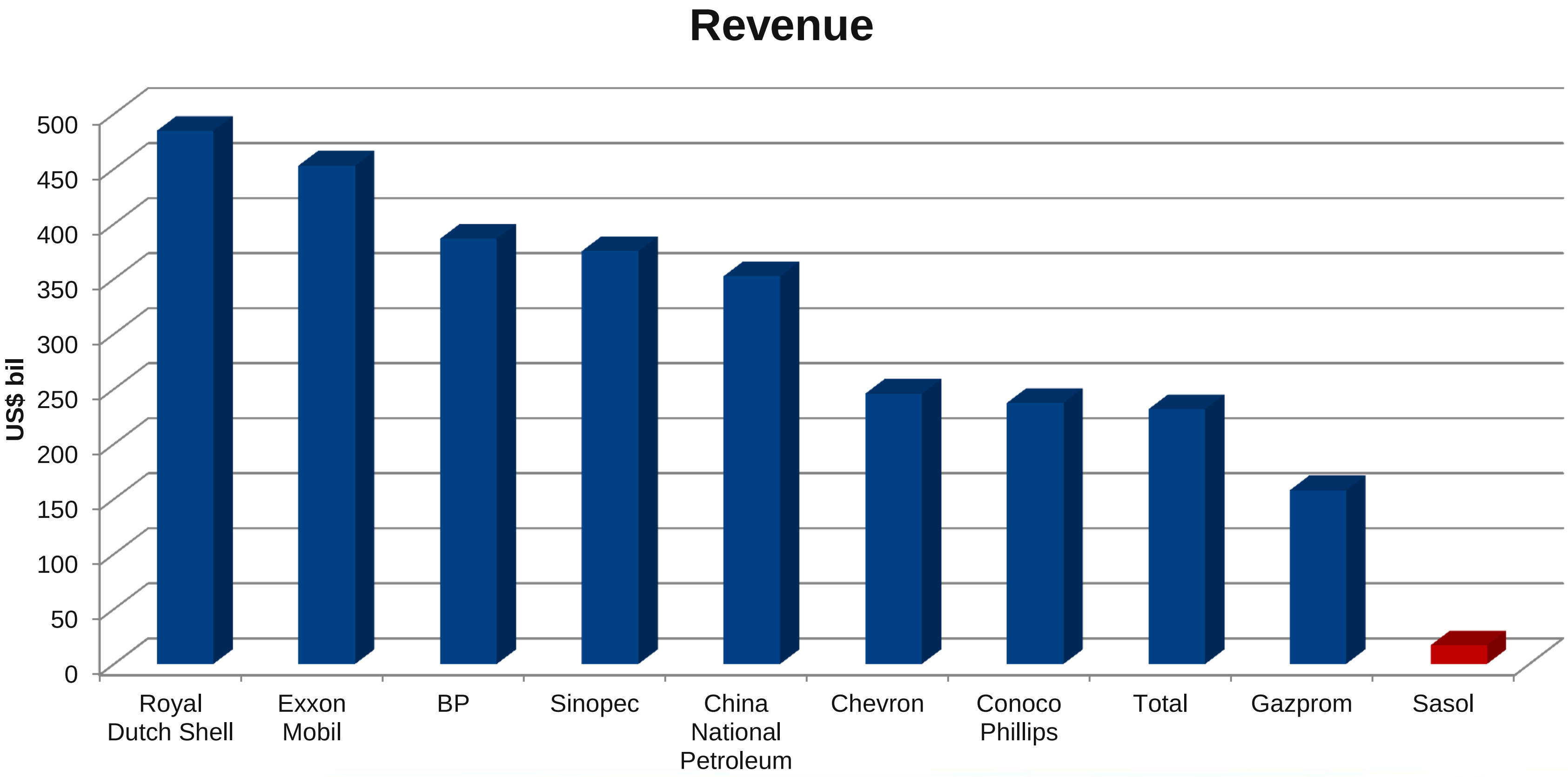
sasol reaching new frontiers

- Established in South Africa in 1950s.
- One of world's largest sole owned petro-chemical complex in Secunda, Mpumalanga:
  - 84 FBDB Gasifiers, 16 Air Separation Units, 9 SAS reactors
  - 160,000 bpd diesel & gasoline
  - 250,000 ktpa co-monomers
  - World-scale polyethylene & polypropylene plant
- Headquartered in Johannesburg, South Africa (JSE and NYSE listed)
- 37,000 employees in 37 countries.
- Owns largest slurry-phase GTL facility in Qatar (34,000 bpd)
- Chemical operations in Netherlands, Italy, Germany, U.S.A, South Africa
- US$ 27 billion market capitalisation (2013)
- US$ 17 billion turnover (2013)

# Sasol global presence


broad indication of Sasol's global presence and of its continuing operations, but is not location-s

# small but growing



***adding value through holistic optimisation***

# *industrial alcohols*

$$(CH_3)\text{-}(CH_2)_n\text{-}OH$$

- commonly produced using *hydroformylation* technology.
- large range of uses

| *purpose* | *n* |
|---|---|
| Solvents | 2..4 |
| Plasticisers | 5..9 |
| Detergents | 10..16 |
| Surfactants | 17+ |

# hydroformylation

- converts olefins to aldehydes and alcohols by reaction with syngas

$$\mathrm{olefin}_{\mathrm{n}} + \mathrm{CO} + \mathrm{H}_2 \longrightarrow \mathrm{aldehyde}_{\mathrm{n+1}} \xrightarrow{+H_2} \mathrm{alcohol}_{\mathrm{n+1}}$$

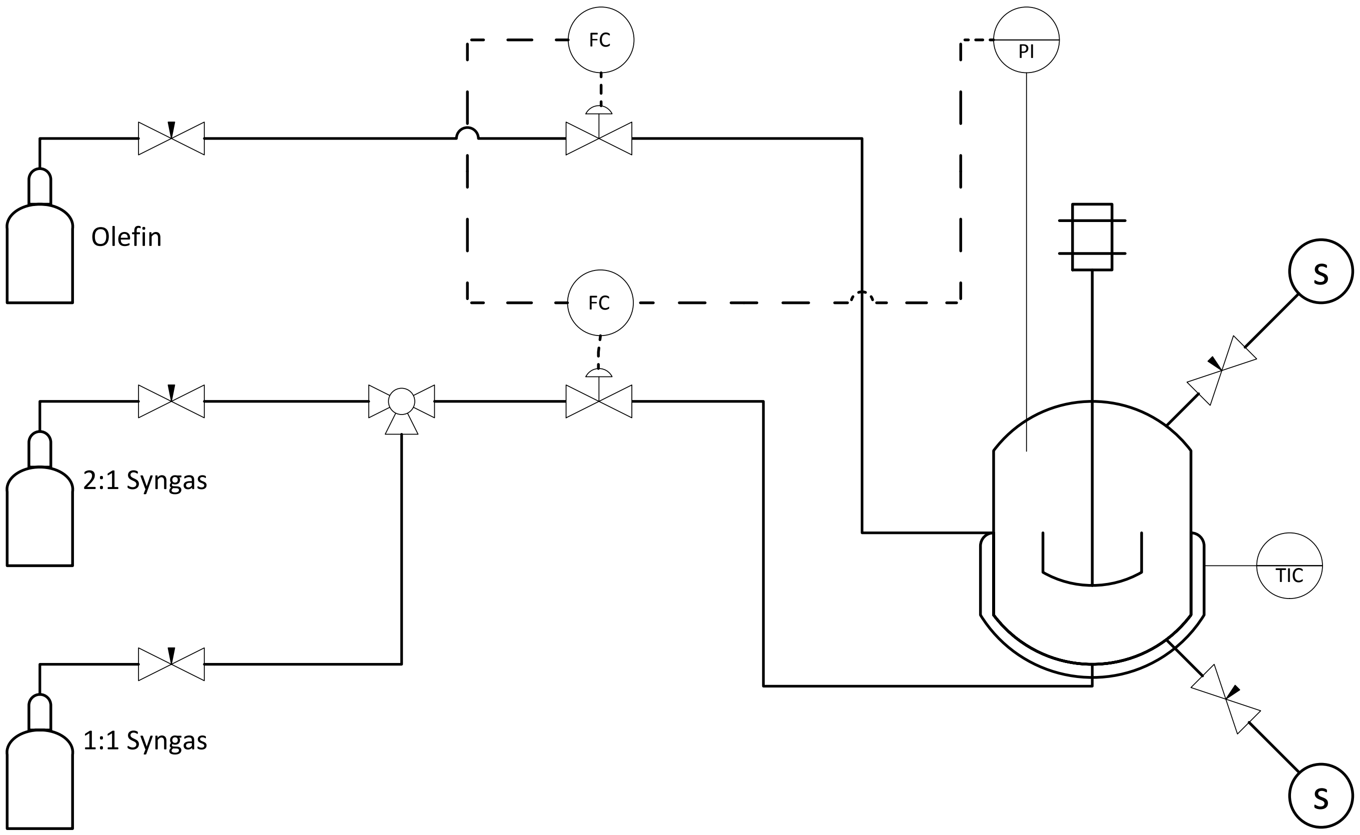
- typically homogeneous reaction, usually catalysed by cobalt or rhodium complexed to a ligand, designed to modify reaction in some manner

# modCo$^{TM}$

- Sasol's proprietary hydroformylation catalyst
- Developed for manufacturing detergent alcohols
- Can be adjusted for producing other industrial alcohols

kinetics

# kinetic apparatus



# *kinetic apparatus*

## Properties

- 1 litre autoclave
- 40 – 80 bar
- 120°C – 180°C

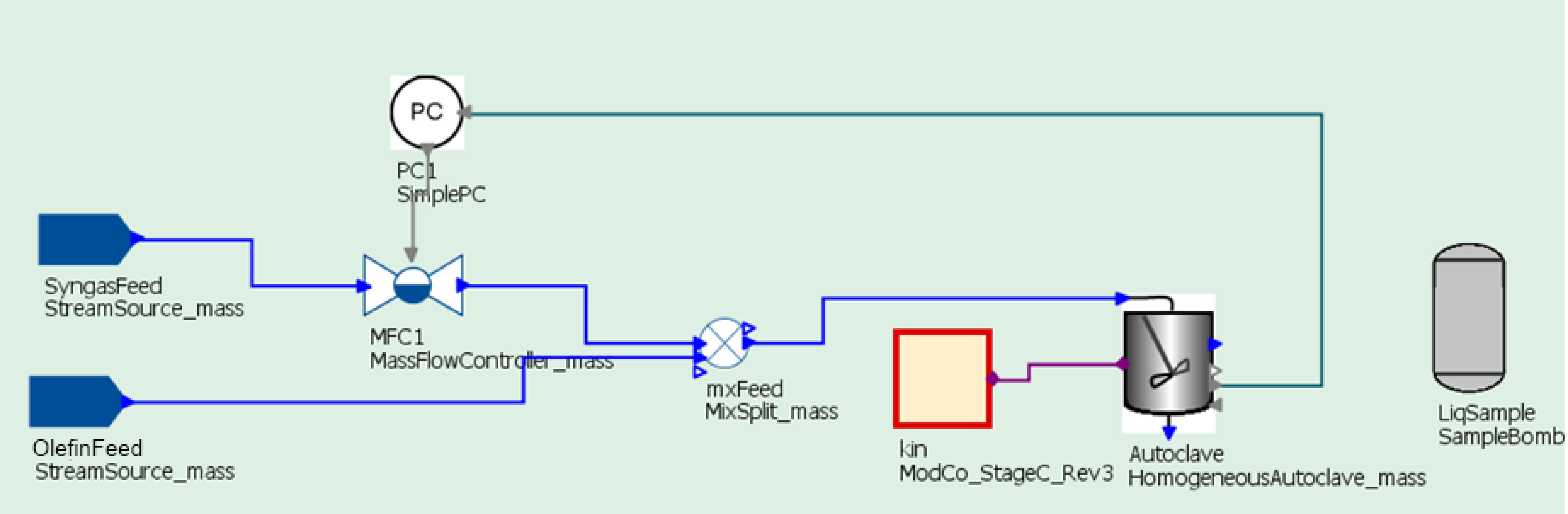
## Feed supply

- olefin and syngas feed, no product line
- feed supplied under pressure and ratio control
- multiple syngas ratios

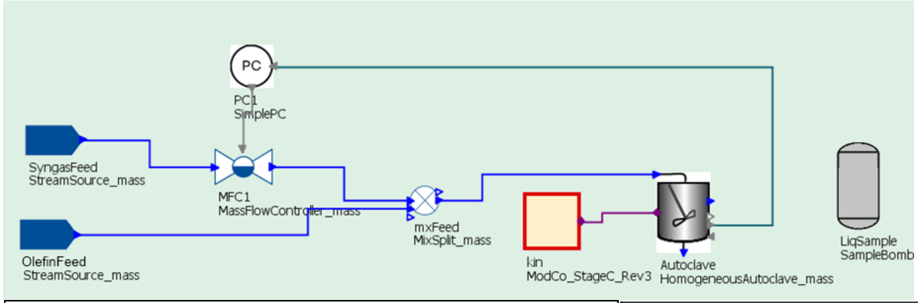
## Data

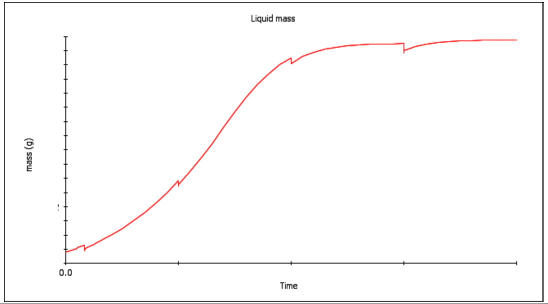
- Inherently dynamic
- Lots of information from single run

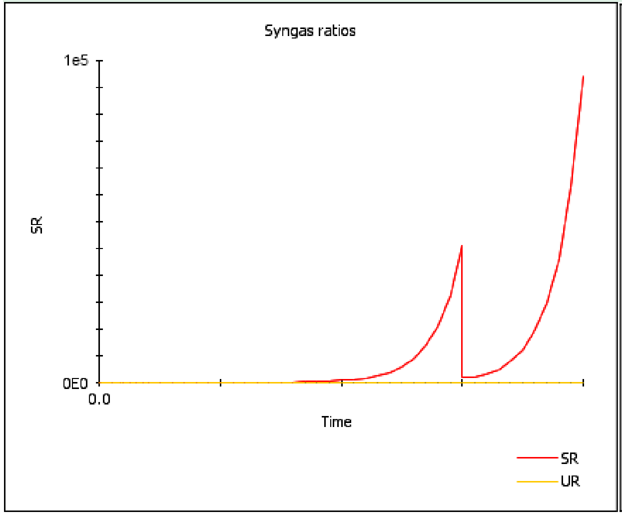
# kinetic rig model

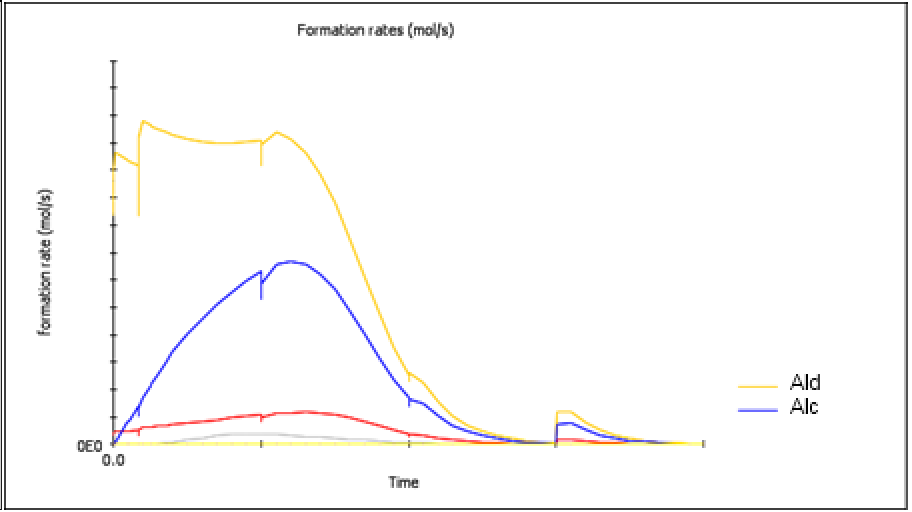


# kinetic rig model sample results

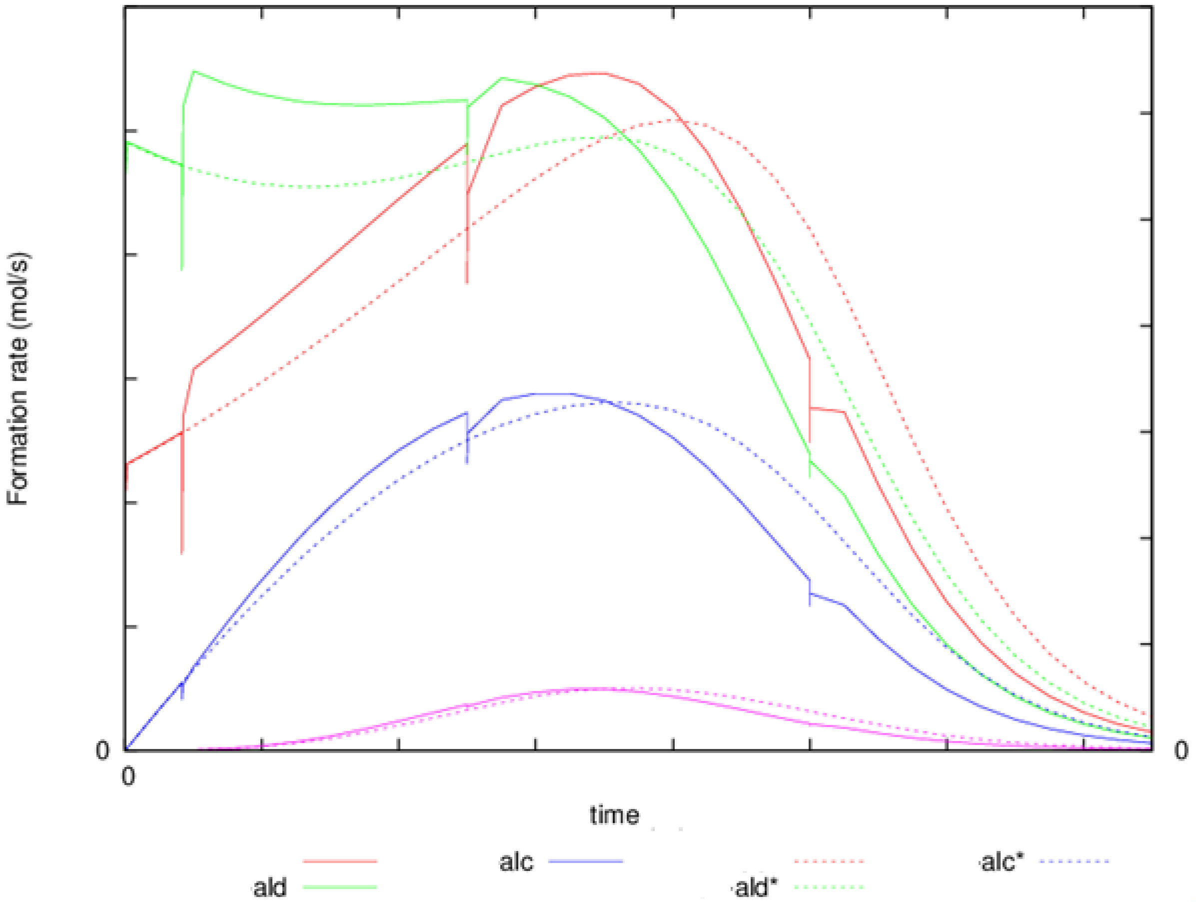


# the effect of sample taking



# kinetic model

sasol
reaching new frontiers

## Concentration terms

- Local liquid concentration determined from EOS
- Solvent agnostic
- Requires binary coefficient data!

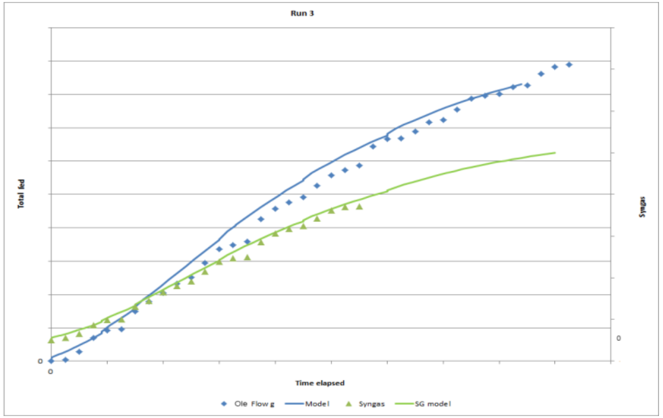
## Catalyst

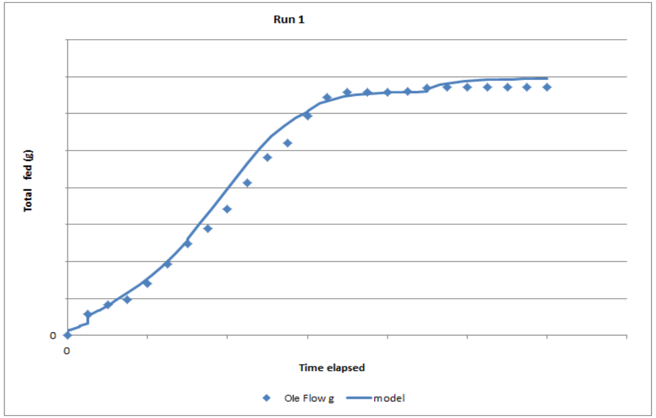
- Complex interplay between multiple catalyst states (e.g. active, dormant and dead)
- Affected by metal, ligand and syngas concentrations

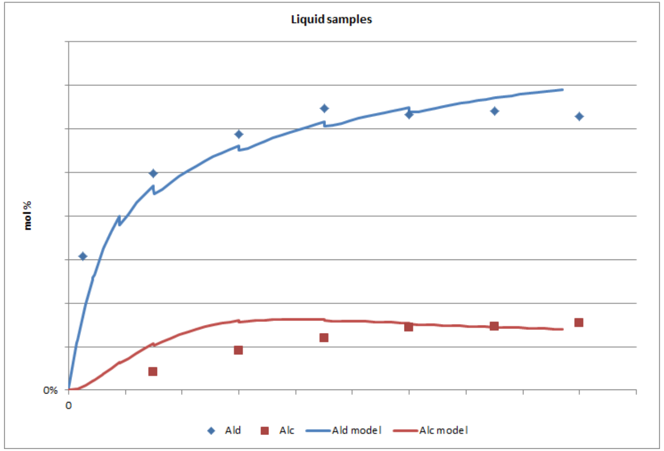
## Reactions

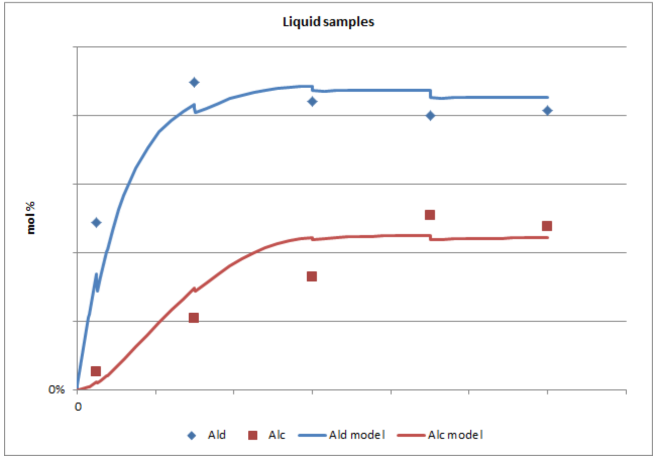
- Primary, secondary and tertiary products
- 16 parameters in total

# *results – kinetic fitting*

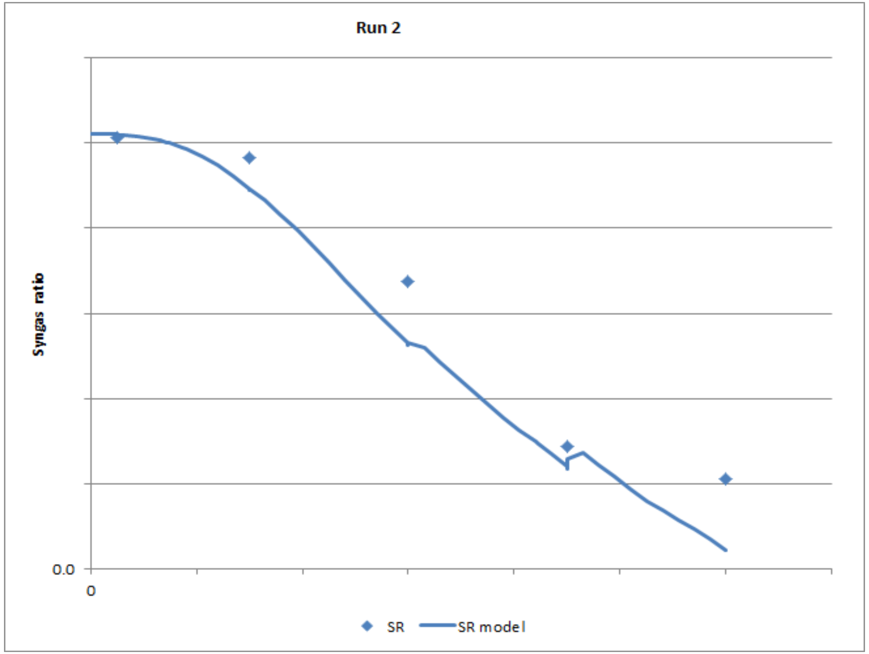


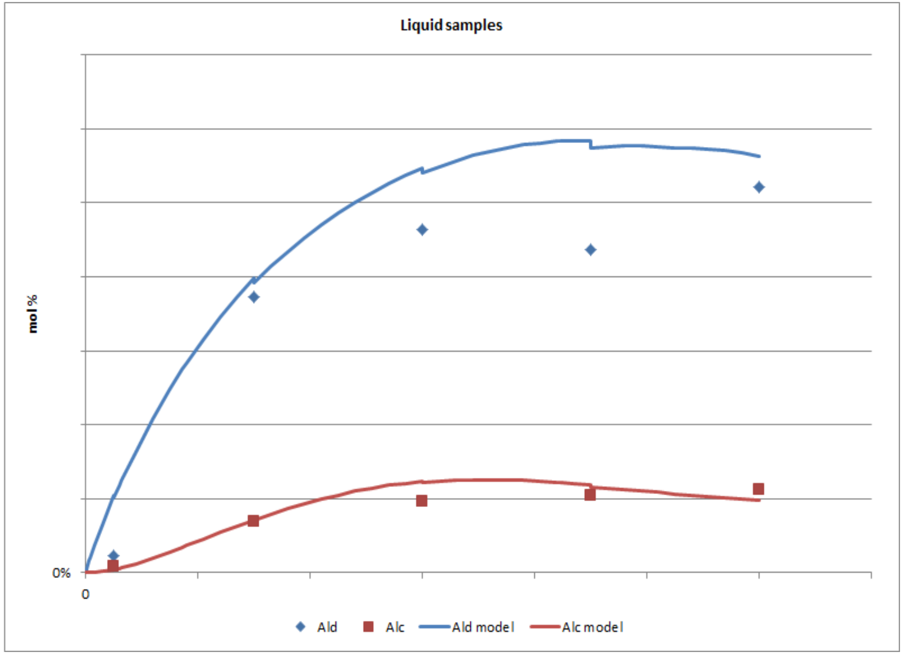



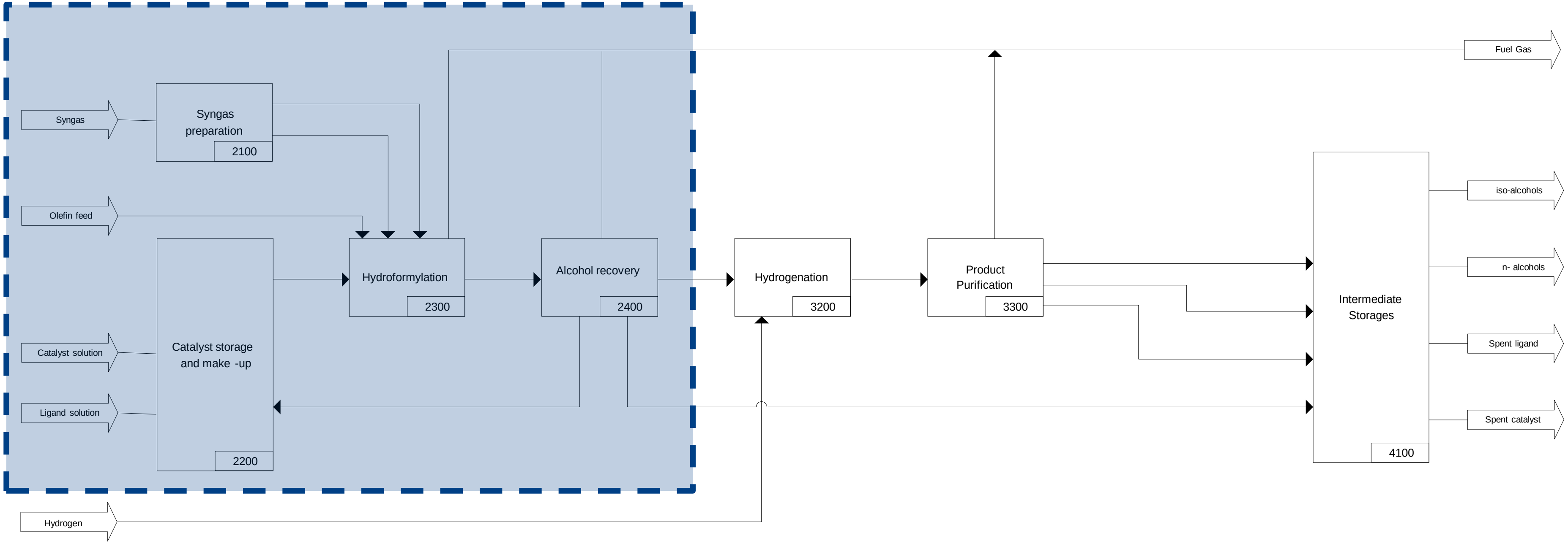
# results - validation



# Process design and optimisation

# block flow diagram



# comparison of holistic vs bau approach

sasol
reaching new frontiers

## business-as-usual

- Steady-state flowsheet design for mass-balance
- Capex and opex done 'over-the-fence'
- Case studies = optimisation

## holistic approach -**"design my plant to maximise return"**

- Mass, energy, utility, capex and opex models integrated into single model.
- Rigorous optimisation with SQP.

## disclaimer and caveats

- Comparison is not scientific or rigorous (too unproductive)
- ~1 week of case studies vs. 2-3 weeks of optimisation studies.

# bau design



## flowsheet

- Copy-and-paste of detergent alcohols design, with some obvious modifications

## equipment design and sizing

- Based on heuristics and rules of thumb

## utility integration

- None

# case studies

## Pressure and temperature

- High pressure, low temperature
- Low pressure, Low temperature

## Contacting strategy

- Counter-current gas flow
- Co-current gas flow
- Varying gas recycle ratio

## Constraints

- Liquid recycle set to maintain catalyst concentration in recycle below limit
- reactor L:D ratio kept at 5.
- Reactor volume varied to achieve >99% C3= conversion.

# holistic approach



## mass balance

- In-house steady-state gPROMS model library
- Kinetics module connected to rigorous bubble column model

## capex

- SRI correlations refitted to internal database
- In-house reactor costing model ported to gPROMS

## opex

- LHV and steam table modules determine value of utility streams
- “Investor” model calculates NPV, IRR, etc. based on given S-curves.

## optimisation

- Maximise IRR, changing key design variables
- Multiple operational constraints (e.g. catalyst concentration)

# *advantages of the holistic approach*

Besides delivering an optimal solution,

Fully examine the parameter space,

providing insight into the process, suggesting additional work on truly *qualitatively different* case studies.

Division of labour

Computers do the boring number crunching

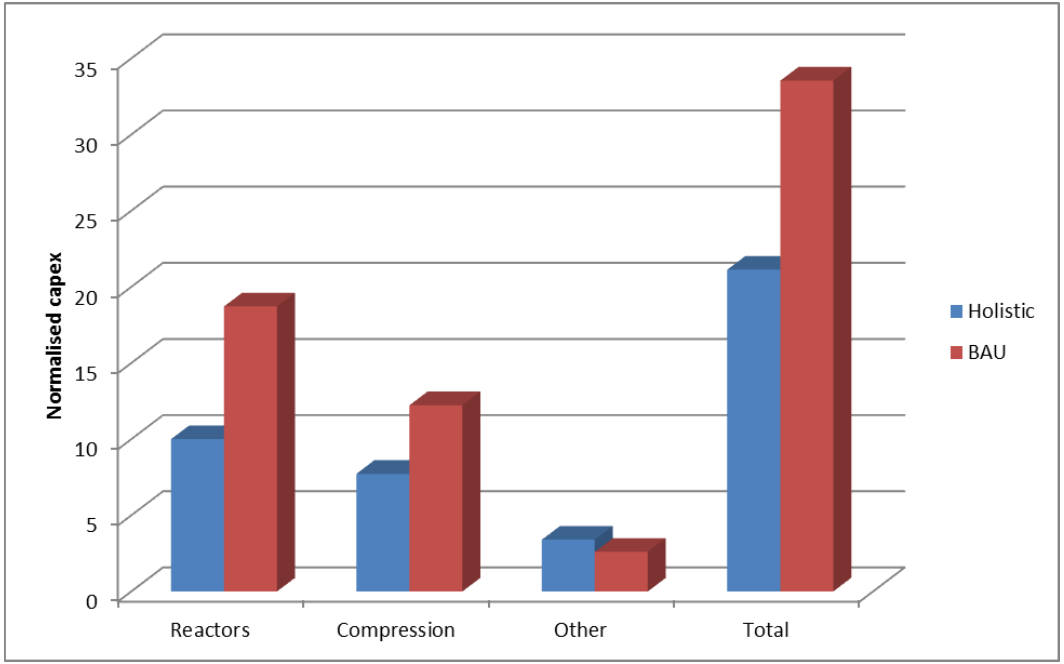
Engineers do the thinking

We get to actually do our jobs

Not a ‘fire and forget’ solution

Time freed up allows for real innovation.

# results - capex




*Capex normalised to $10million for reactors in holistic flowsheet

# results - production

## process efficiency

- Byproduct yields in BAU design made process non-viable.
- Alcohol yields > 90% found in holistic case, though economic optimum was less than this.

## breakthroughs

- design change “A” led to lower operating pressure, significantly saving compression costs
- relaxing heuristic assumptions and rules-of-thumb led to dramatic capex savings, particularly in reactors.
- energy optimisation led to lower overall capex while simultaneously improving reactor productivity.
- Constrained syngas management optimisation led to dramatically improved yields

# conclusions

artificial example – 37% capex savings

- In general, 20% capex savings is realistic, and additional opex savings due to energy integration optimisation.

Inclusion of utilities & economics into `super-design' opens up integration synergies that are impossible with '1-at-a-time' or 'over-the-fence' approaches

gPROMS is a tool that facilitates and enables holistic design and optimisation, from the lab scale through to conceptual design

sasol
reaching new frontiers

***Holistic optimisation***
*An industrial case study*

better together...we deliver