The INCOOP Methodology applied to the Shell Case Part I Modelling and Simulation

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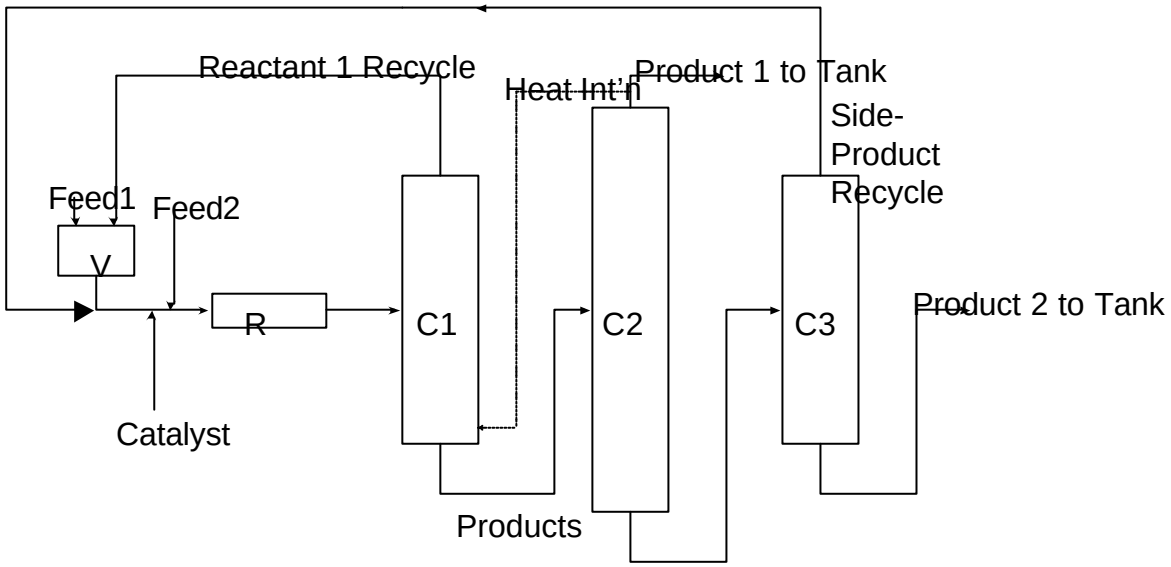
Simplified Process Flowsheet



Full model size

- # units: two dozen
- # variables/equations: 10-20k
- # differential equations: 1k-2k
- Time constant: hours & mins

Full model challenges

- Combined lumped, staged, distributed
- 2x recycle, heat-integration, 20-40 control loops
- Level of detail

Example part of Mathematical Model

$$\frac{\partial C_i(z,t)}{\partial t} = -\frac{\partial F_{c,i}(z,t)}{A\partial z} + \Sigma_j n_{ij} r_j(z,t) \text{for} \forall\ i$$

$$F_{c,i}(z,t) = Av(z,t) \times C_i(z,t) \text{for} \forall\ i$$

$$Av(z,t) = V_{liq}(T(z,t), 10^5 P(z,t), F_{c,i}(z,t)) 10^3$$

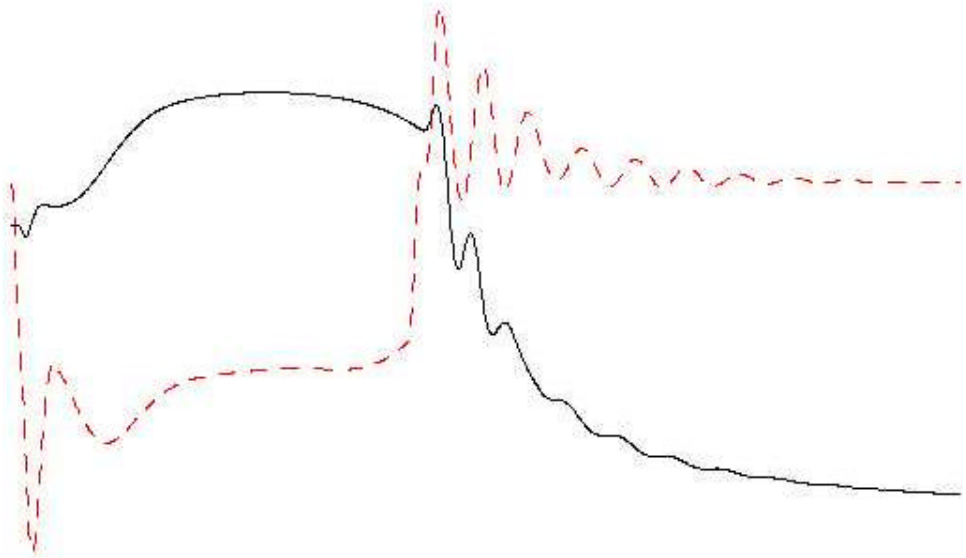
In tubular reactor::

- C are concentrations
- F are flows
- r are reaction rates
- v is velocity
- V_{liq} is specific liquid volume

Note

- use of flows (calculation time)
- propriety physical properties
- scaling
- implementation in gPROMS

Example simulation



Response to step change in feed on (red dashed) level in condenser and (black solid) a potentially observable temperature in reactor

Towards Optimal Complexity

- Avoiding theoretical shortcuts including kinetic energy terms in energy balance in reactor.
- Adding theoretical requirements: pressure drop in liquid phase reactor ie the momentum balance.
- Adding practicalities: finite mass of mixers and reactor wall which could induce short time constants.
- Adding existing controllers in mixers.
- Extreme cases with discrete event modelling such as full trays.

Actual choice:

- No kinetic energy terms: caused conflicts in equation oriented environment.
- Retained pressure dependence as it did not affect computation time much.
- Removed finite masses: difficult to estimate and significantly reduced computation time.
- Removed mixer controllers: robustness
- Retained discrete events: normally not effective.

Criteria and tests:

- steady state initialisation, robustness with respect to different initial values – state re-initialisation.
- Performance of required step change on feed and a complete trajectory over days – range of operation for optimisation.

Implementation bottlenecks

Modelling environment: gPROMS with propriety physical properties package.

- Number of *relevant* components in separation unit much less than in conversion unit. Equation-oriented package is not flexible for this.
- Initialisation (and possible future reinitialisation) was constantly a point of consideration. It was achieved with a single start point of all 15k variables, although – after considerable effort – a limited set of 2k proved sufficient, in a specific case.
- The implementation of discrete events was at times necessary, however the optimisation users of the model were requiring a model with at maximum one discontinuity.
- The tuning of the control loops proved a challenge. Because of the high degree of coupling in the system, the standard tuning estimates were inadequate.
- The attempts to model a grade change all faltered possibly because of the high demand on computer resources.

Model validation

There were a number of tuneable parameters in the system:

- A scale factor representing the catalyst activity.
- A constant describing the friction of flows in the columns.

Experience and analysis of several sets of data showed

- That a set of flow measurements could not be reconciled.
- That variation in the catalyst feed composition occurred and that could be adequately described with a first order system.

Some ten parameters were estimated. Then still some temperature profiles differed by 10% (of the total temperature range in the system) from reality. It is likely that the used laboratory data were insufficient to model at this scale.

Alternative: use of wavelet decomposition to characterise data and simulation and compare as wavelets: timescales better represented.

Model validation – wavelet decomposition

Figure with wavelet from JPS completely scaled

Liquid phase reactor

$$\frac{\partial \boldsymbol{C}}{\partial t} = -\frac{\partial \boldsymbol{F}}{A\partial z} + \Sigma_j \boldsymbol{n}_{ij} r_j(\boldsymbol{C})$$

$$\boldsymbol{F} = A v \boldsymbol{C}$$

$$1 = \boldsymbol{C}^t \boldsymbol{V}_{liq}$$

Vectorial form

- F, C and v are variables
- Constitutive equation: no independent choice of differential variables.
- High-index problem connected with volume constraint

... But gPROMS simulates in total system!

Effect only found there where the sensitivity equations were applied: the sensitivity matrices are highly singular. This affected the optimisation and the control algorithms.

For control simplified reactor model used circumventing volume constraint

... But are there other – rigorous – solutions?

The INCOOP Methodology applied to the Shell Case Part II Control and Optimisation

Shell: Piet-Jan Brouwer, Sjoerd de Wolf, Celeste Colantonio

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TU Eindhoven: Mario Balenovic, Andrej Tiagounov

RWTH Aachen: Martin Schlegel, Jitendra Kadam

TU Delft (S&C): Dennis van Hessem, Jogchem van den Berg, Adrie Huesman

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Content

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2. Observer
3. Model reduction
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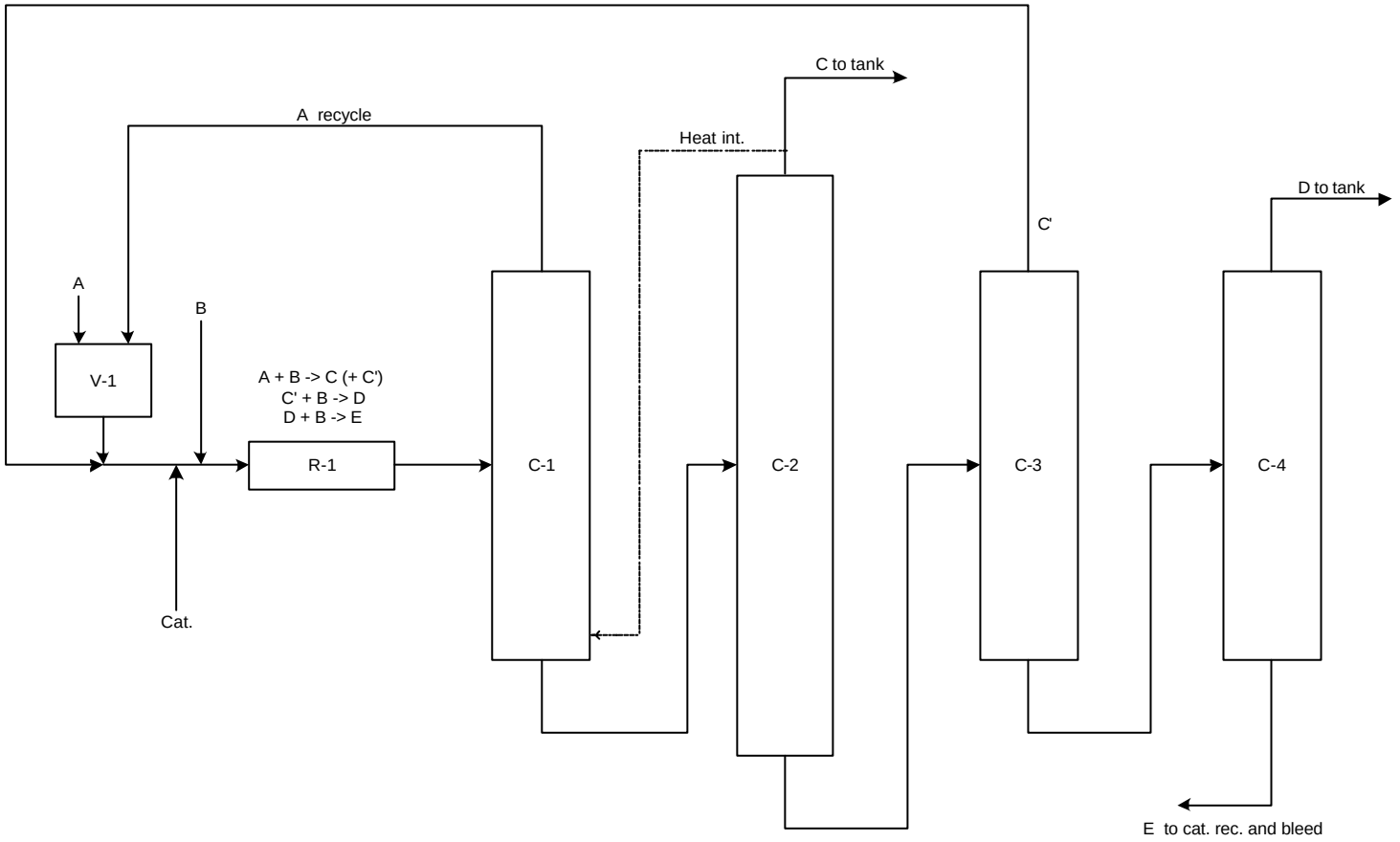
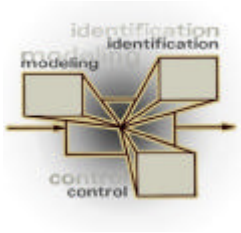
5. Dynamic Optimization
6. Conclusions

Basic Control: Material Balance Control



The production rate is set by the flow of B to R-1. A and cat. are set in ratio with B. After R-1 rate changes are propagated by the level controllers in the bottom of each column (push scheme).

Basic Control: Quality Control



•To make sure R-1 achieves full conversion the inlet temperature is controlled as well as the Delta T over a part of R-1 by cat. ratio.

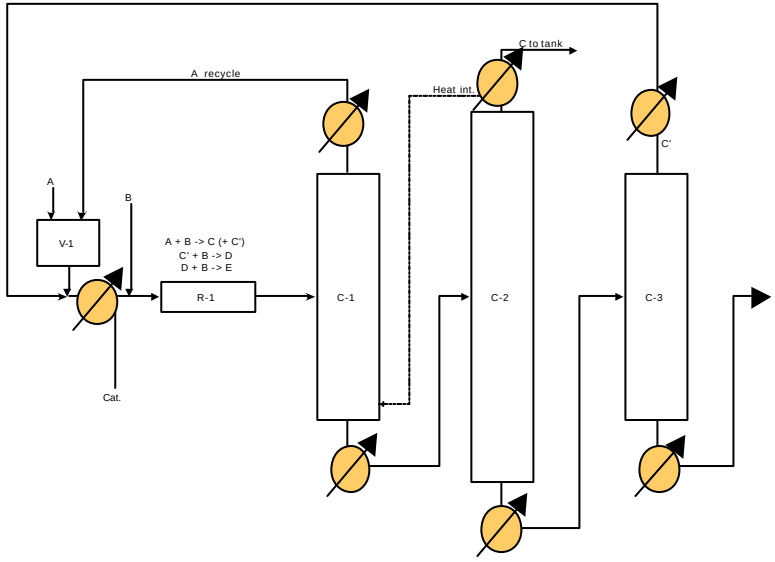
•The compositions of all distillate flows are analyzed by GC's, but the results are not used in closed-loop control. The control of the Split and Sharpness of fraction is given below.

	C-1	C-2	C-3	C-4
Split	temperature by reboiler duty	ratio distillate/feed	temperature by reboiler duty	temperature by reboiler duty
Sharp. of frac.	reflux	reboiler duty	reflux	reflux

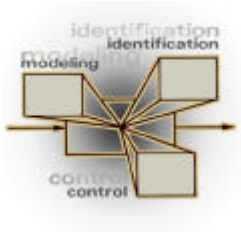
Observer: Type & Definition

Type: Extended Kalman Filter

- Control sample time 10 min,
- Estimation sample time 5 min.
- 1100 states: 90% components in the system
- 40 measured outputs:
  - Mainly focused on flows and qualities
  - Temperatures difficult to connect to theoretical trays



$$\varnothing = (F_i, c_i)$$



2 stage model reduction technique

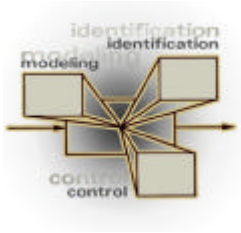
Physically:

- components on connected trays,…
- PDE in tubular reactor model,…

Mathematically:

- Fixed projection reduces states 1100 to 500
- Input-output balanced truncation red. states from 500 to 50+
- Both methods use the local dynamics on-line
- Reduction needs analysis and is not automated
- Reduction also needs dedicated numerical tools (here combination of own software with SLICOT routines)

Observer: Speed



•Results: Just the observer (without MPC) has an execution period of 1 - 2 minutes on a Pentium 4 PC (2 GHz, 1 Gb RAM).

• Computation time is divided over:

  • Model initialization and integration over 2 time steps (LARGER PART,80%)

  • Communication GPROMS-OPC-MATLAB

  • On-line model reduction and linear algebra (time~nx^3)

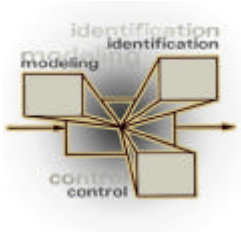
  • Line–search if GPROMS fails to initialize on state update(seldom)

  • QP if constraints are defined

Model Reduction

• Compute Jacobian of the model	$\dot{x} = f(x, y, u)$ $0 = g(x, y, u)$
• Derive linear model	$\Delta\dot{x} = A\Delta x + B\Delta u$ $\Delta y = C\Delta x + D\Delta u$
• First reduction linear model with fixed projection *(e.g. remove connectivity)*	$\Delta\dot{z} = \tilde{A}\Delta z + \tilde{B}\Delta u$ $\Delta y = \tilde{C}\Delta z + D\Delta u$
• Second reduction on reduced linear model by balanced truncation (online)	$\Delta\dot{z}_b = \hat{A}\Delta z_b + \hat{B}\Delta u$ $\Delta y = \hat{C}\Delta z_b + D\Delta u$

Model Predictive Control: Type & Definition

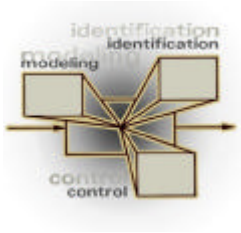


•Type: Input-output MPC (LTV approach) solved as a QP. The numerical integration of the non-linear model is computationally the most expensive part. This resulted in a short time horizon (300 minutes), but compensation was provided by end-point weighting.

•Definition: The CV's are chosen based on process economics, constraints and operational issues. This results in 8 CV's:

Number	Name	Type
1	Relative D production	Set point
2	Top quality C-1, A	Set point
3	Top quality C-2, A	Set point
4	Top quality C-2, C'	Set point
5	Top quality C-3, C	Set range
6	Top quality C-3, D	Set point
7	Top quality C-4, C'	Set point
8	A recycle	Set range

Model Predictive Control: Definition



- The MV's were selected such that there is adequate control over the CV's (see below).
- In general CV's 5 and 8 do not require any MV's so normally the application is "square" (6 by 6).

Number	Name
1	Reboiler duty C-1
2	Reflux C-1
3	Ratio distillate/feed C-2
4	Reboiler duty C-2
5	Reboiler duty C-3
6	Reflux C-3

Model Predictive Control: Reduction & Results

•The model reduction is as discussed before (for the end-point weighting).

•Results: Just MPC (without observer) has an execution period of 4 minutes on a Pentium 4 PC (2 GHz, 1 Gb). So including observer an execution time of 10 minutes is possible.

Dynamic Optimisation

- Type: Sequential approach dynamic optimisation
- Task: Faster, more efficient load change
- Challenges:

  - size of the model: > 12,000 differential-algebraic equations

    ⇒ much larger than Bayer Case, can be handled by implementation

    ⇒ numerical state and sensitivity integration is slow due to size model

  - model reduction not applicable in this context

    ⇒ higher computation time, less accurate

- Successfully applied to subset of the plant (distillation column with 2750 equations) ⇒ faster load change achieved

Conclusions

•Despite improvements in the environment modelling remains labour intensive requiring experience, know-how etc..

•Simulation of the non-linear model is 2-10 faster than real-time (depends on type of inputs and the way they are communicated).

•The hybrid model is an adequate representation of the plant.

•Model reduction has proved to be a more difficult issue then anticipated. The computational effort also depends at least on the solver and there is a trade-off between speed and accuracy.

•Simulation of the non-linear model explains for the major part of the computational effort.

•Using model reduction first, the developed extended Kalman filter and MPC are able to work real-time for the Shell Case.