ADVANCED PROCESS MODELLING FORUM
LONDON
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Online Model-based Applications (OMBAs)

Real-time monitoring of ethylene cracking furnaces

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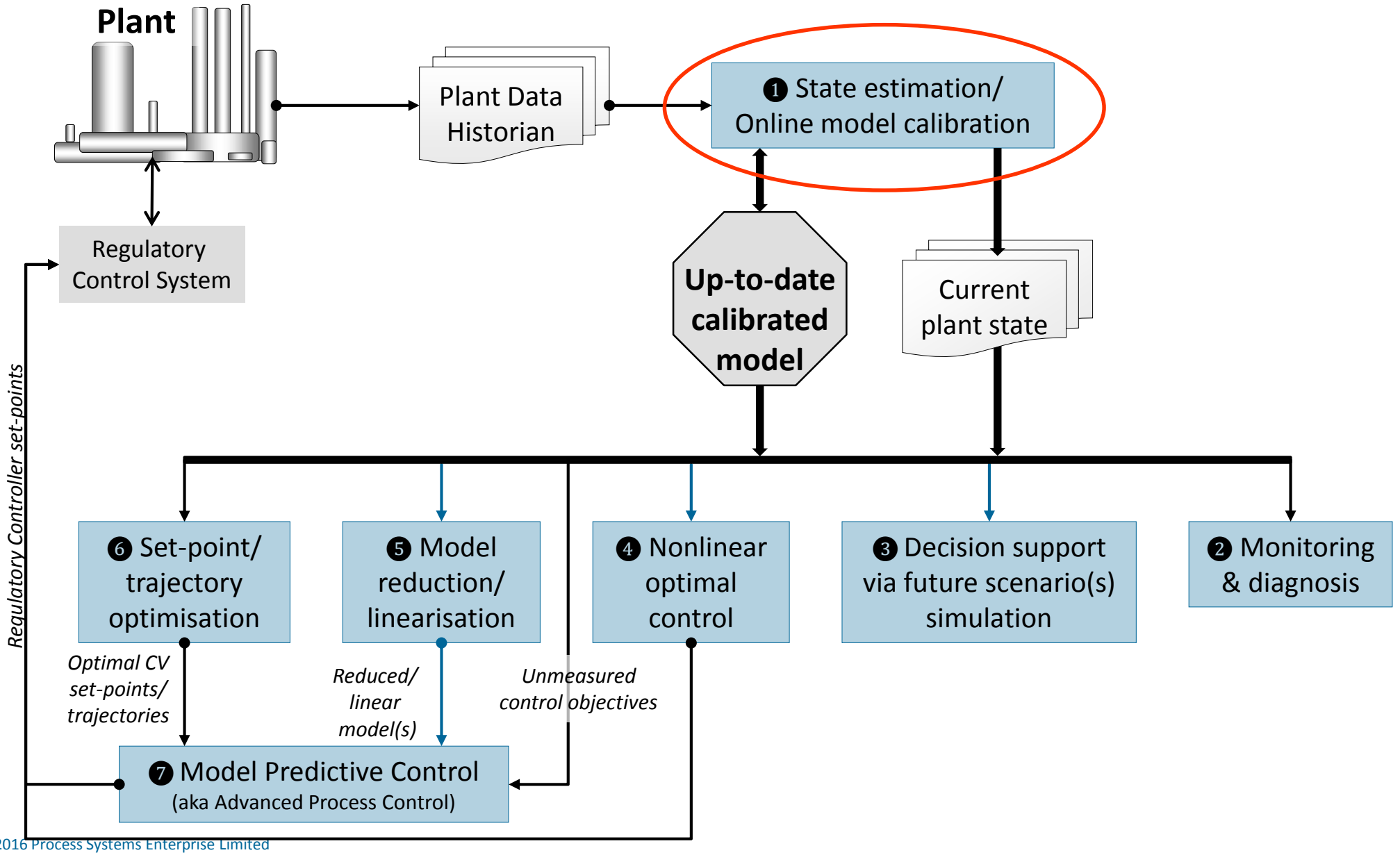
gPROMS

Online Model-Based Applications (OMBAs)

Integrated framework – the 'big picture'

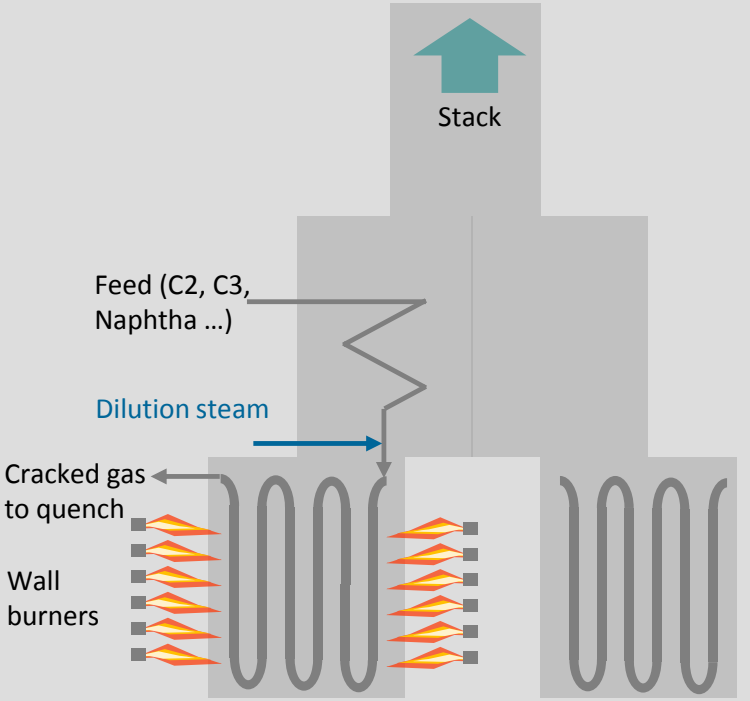


Background

Steam crackers

- Large, complex units at heart of petrochemical complexes
  - produce key building blocks: ethylene, propylene, butadiene, aromatics, acetylene
  - furnaces crack hydrocarbon feedstocks in the presence of steam
  - temperatures between 800–860°C
  - continuous coke deposition in coil, TLE and quench

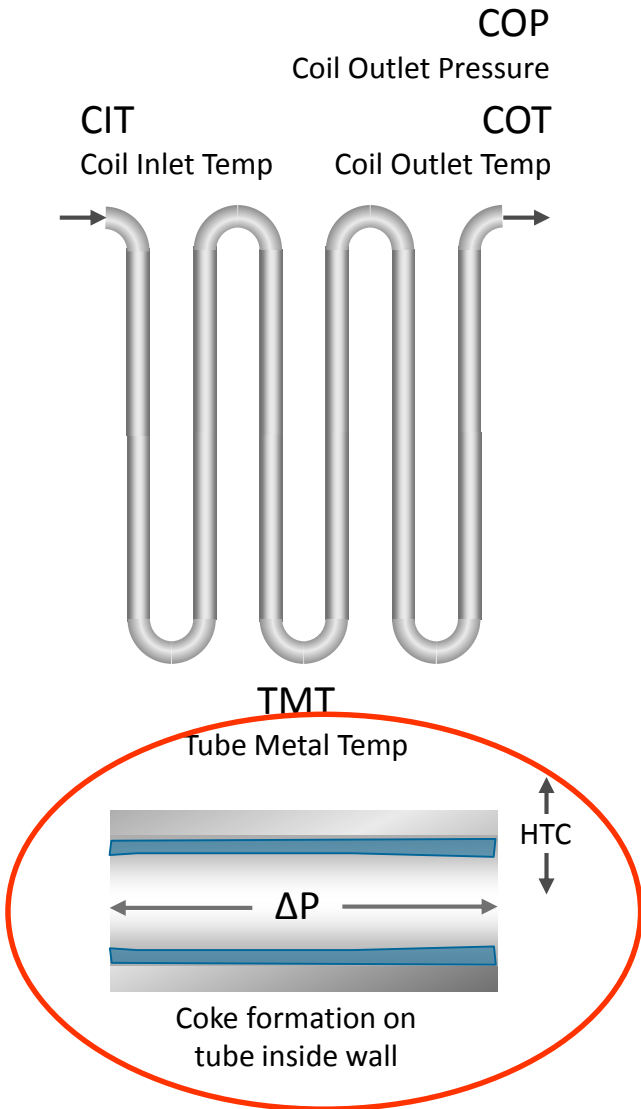
➔ MAJOR CHALLENGE: predict rate of **coking** and effect on performance, particular yield prediction



The challenge of coking

- Coking
  - occurs along length of coil
  - can be exacerbated by changes in operation (feed flowrate, steam, etc. fluctuations)
- Effects increase over time
  - reduced heat transfer
  - increase in metal skin temperature
  - increasing pressure drop
- Operations interrupted for decoking
  - depends on feedstock, operating conditions
  - triggered by pressure drop (small diameter tubes) or metal temperature (larger tubes)
  - typically 60-90 days

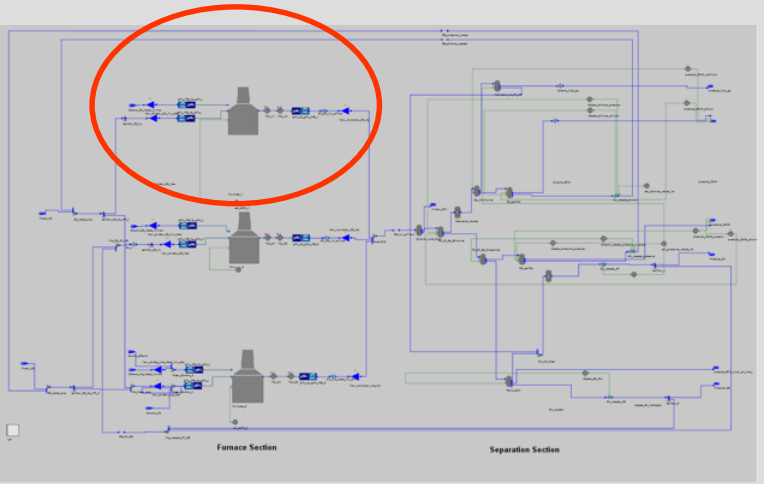
Key variables

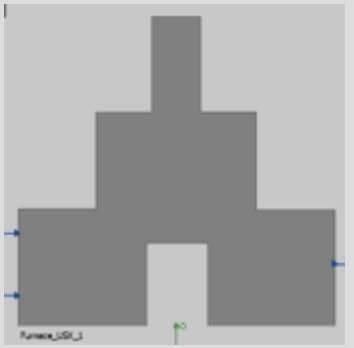


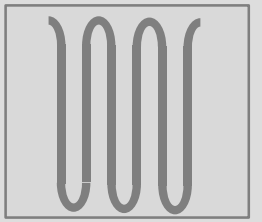
Approach

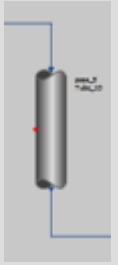
Model-based approach

- First-principles model of furnace
  - modular, hierarchical models
  - multiscale, distributed
- Evolving gPROMS ProcessBuilder Olefins library



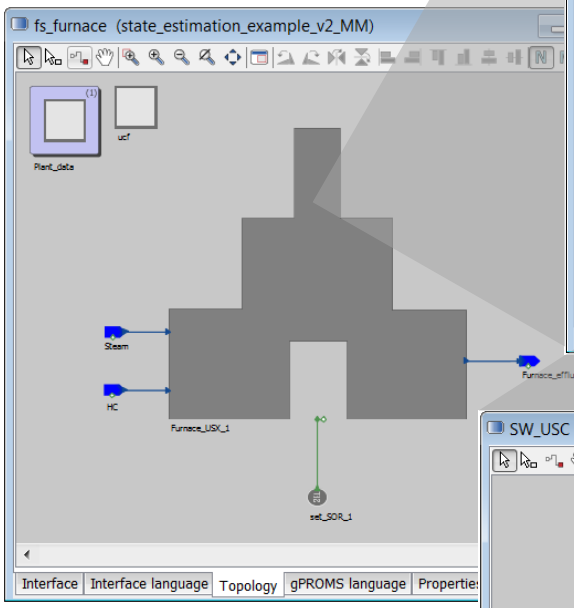




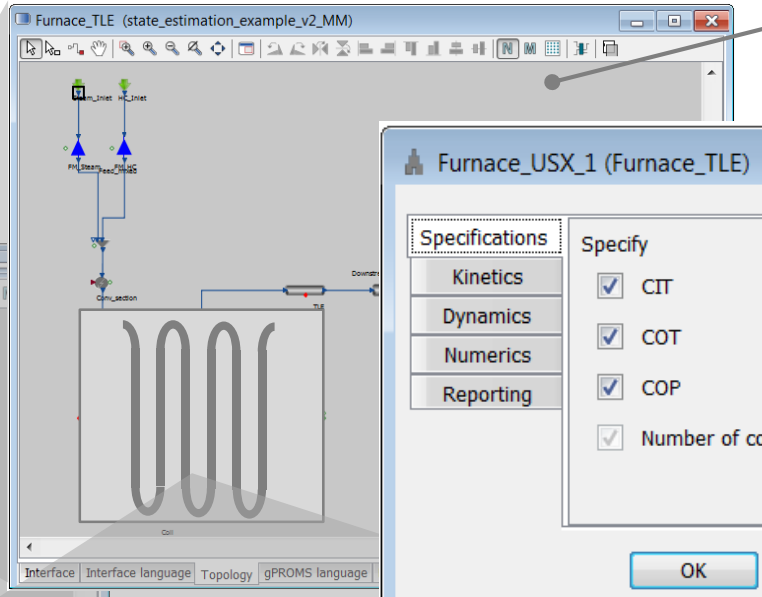


Furnace/coils – geometry

Furnace

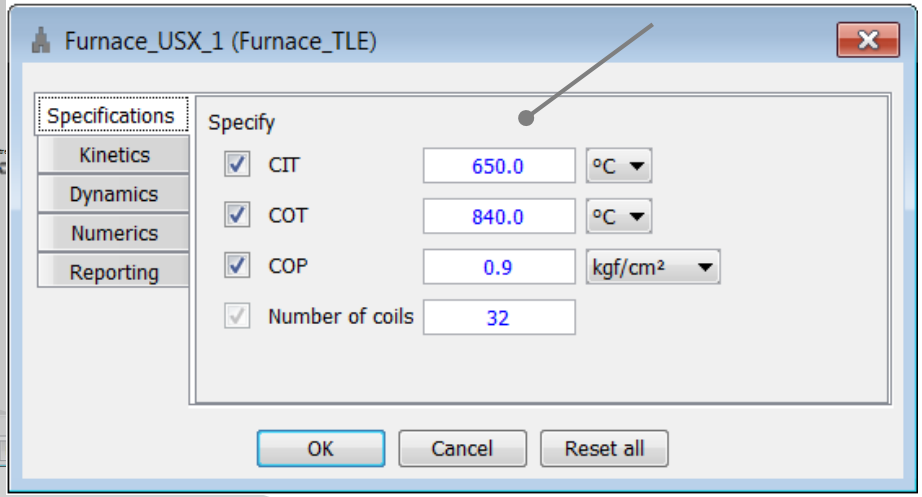


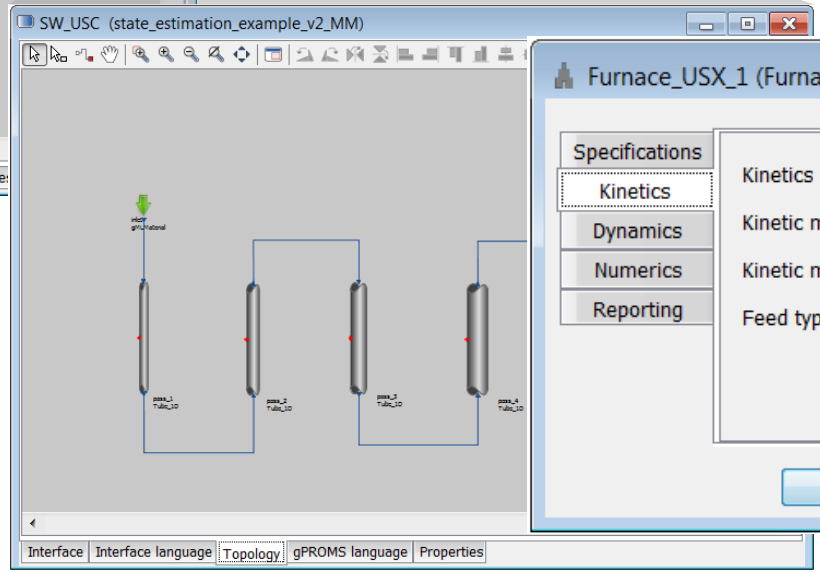
Can be used for different geometries, feedstocks



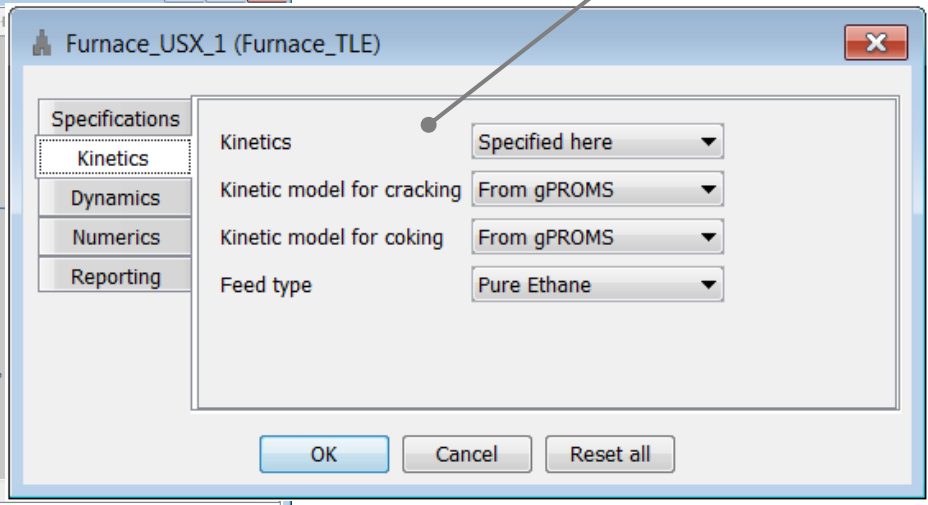
Coil & transfer line models

Overall furnace spec





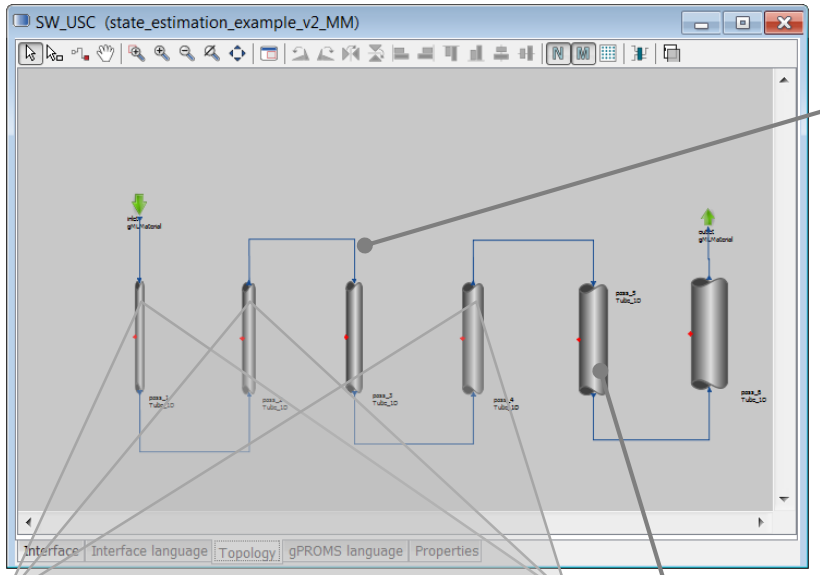
Kinetics defined at top level

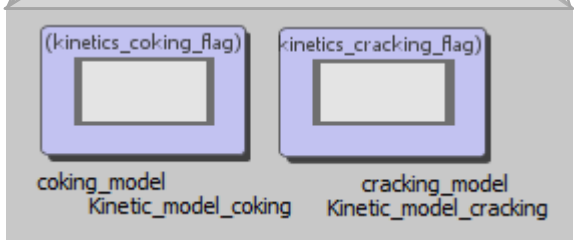


Furnace/coils – geometry and kinetics

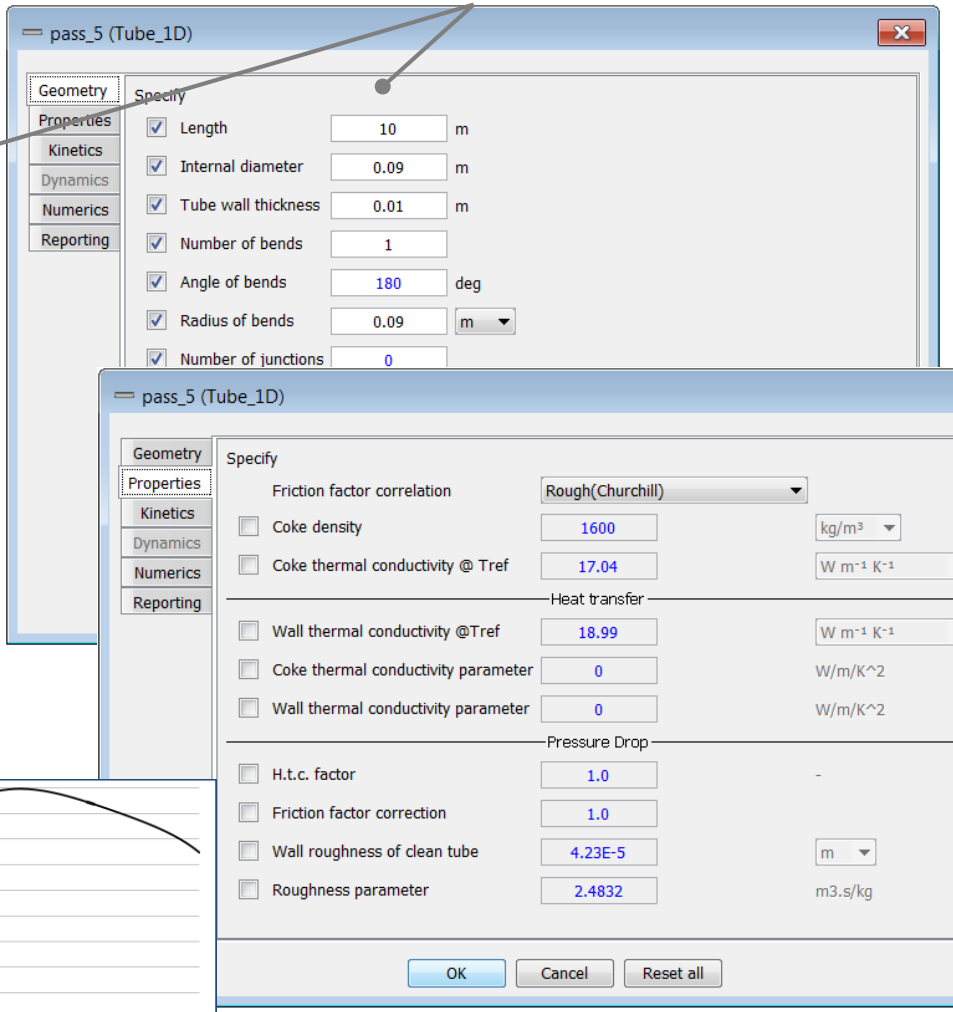
Coil

Any coil configuration possible – take into account geometry

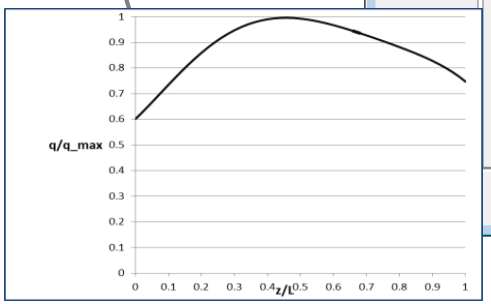




Cracking and coking kinetics models – 'inherited' from top level but can differ per segment



Coil pass properties

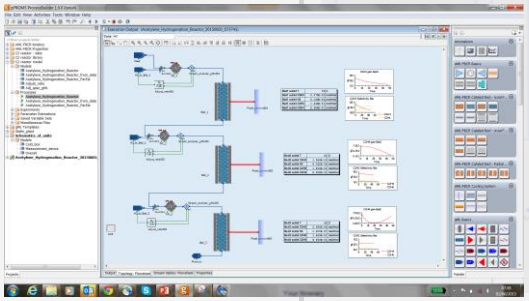


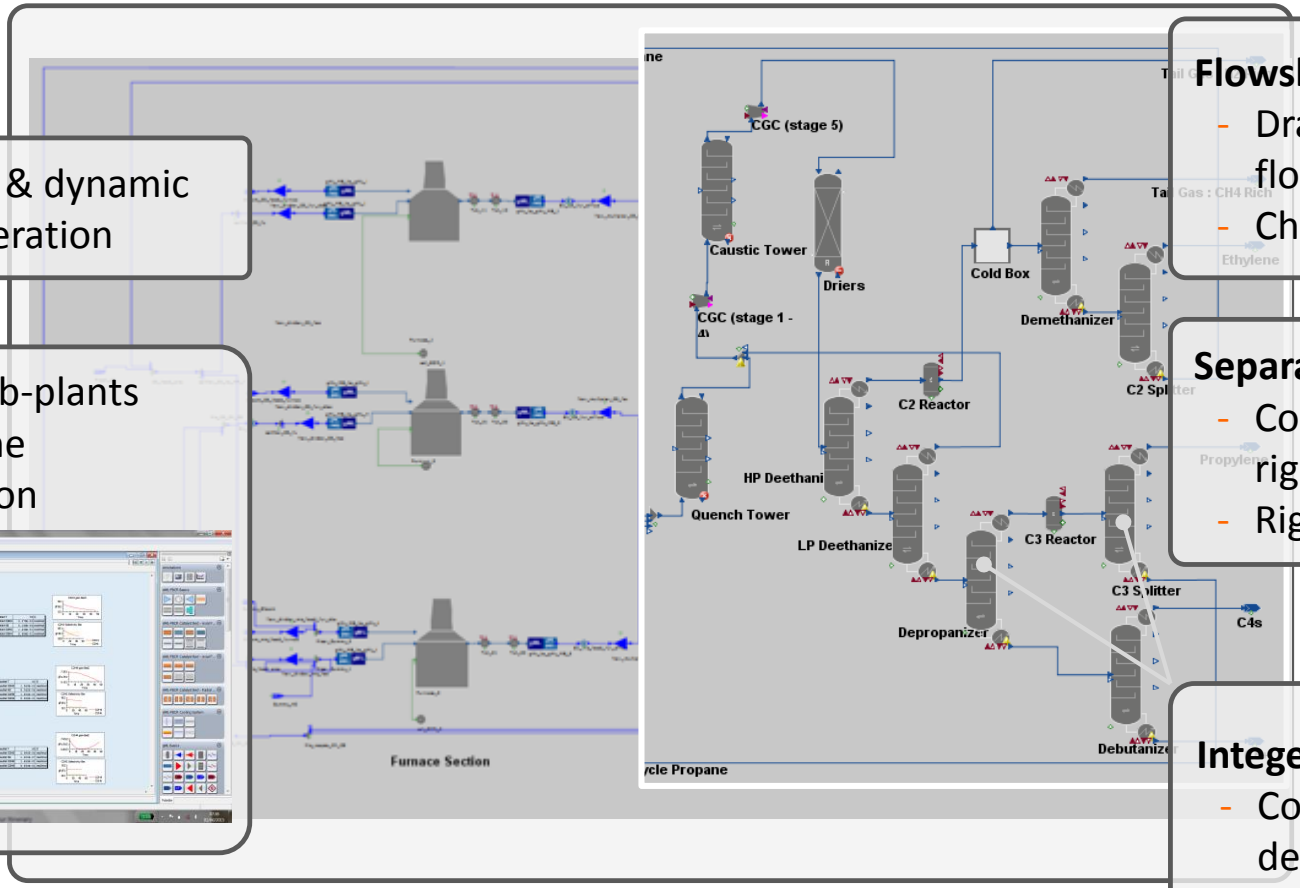
Relative heat transfer profiles

Wider context – whole plant
Typical application

- Steady-state & dynamic
- Design & operation

Can include sub-plants
- E.g. acetylene hydrogenation





Flowsheeting environment
- Drag & drop flowsheeting
- Choose fidelity level

Separation
- Component splitter or rigorous column
- Rigorous thermo

Integer optimisation
- Column configuration decisions (e.g. feed tray location)
- Column order / process routing

- Can include any sub plant
  - E.g. acetylene hydrogenation, compression, …
- Any level of complexity

Kinetics models

Reaction kinetics

Cracking model

Reaction #	Reaction rate
1	$R_1 = k_1[C_3H_8]$
2	$R_2 = \vec{k}_2[C_3H_8] - \frac{\vec{k}_2}{K_{eq,2}}[C_3H_6][H_2]$
3	$R_3 = k_3[C_3H_8][C_2H_4]$
4	$R_4 = k_4[C_3H_6]$
5	$R_5 = k_5[C_3H_6]$
6	$R_6 = \vec{k}_6[C_3H_6] - \frac{\vec{k}_6}{K_{eq,6}}[C_2H_2][CH_4]$
7	$R_7 = k_7[C_3H_6][C_2H_6]$
8	$R_8 = \vec{k}_8[C_2H_6] - \frac{\vec{k}_8}{K_{eq,8}}[C_2H_4][H_2]$
9	$R_9 = \vec{k}_9[C_2H_4][C_2H_2] - \frac{\vec{k}_9}{K_{eq,9}}[C_4H_6]$
10	$R_{10} = k_{10}[C_2H_4][C_2H_6]$

Reference: Sundaram, K.M., & Froment, G.F. 1977. Modeling of thermal cracking kinetics – I : Thermal cracking of ethane, propane and their mixtures. Chemical Engineering Science, 32, 601{608.

$$k_i(T) = k_i(T_{ref}) \exp\left(-\frac{E_a}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right)$$

Reaction kinetics
Coking model (dynamic)

- Mass continuity equation for coke:

$$\frac{dm^{coke}(z)}{dt} = \frac{2R_i(z)}{R_W^2} r_{coking}(z)$$

Coking rate:

Influential — Very influential — Not influential — Not influential

$$r_{coking}(z) = k_{c1} c_{C_2H_4}(z) + k_{c2}\left(\frac{c_{C_2H_4}^2}{c_{C_3H_6}}\right) + k_{c3} c_{C_3H_6} + k_{c4} c_{1-3but.}$$

with

$$k_i(T) = k_i(T_{ref}) \exp\left(-\frac{E_{a,i}}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right), \qquad \text{i} = \text{c1, c2, ...}$$

Wauters, S., & Marin, G.B. 2002. Kinetic Modeling of Coke Formation during Steam Cracking. Ind. Eng. Chem. Res., 41, 2379{2391
Albright, L.F. 2002. Comments on 'Kinetic Modeling of Coke Formation during Steam Cracking'. Ind. Eng. Chem. Res., 41, 6210{6212
Plehiers et al (1990).

Reaction kinetics

Coking model implementation

- Implemented as a custom kinetics model

Kinetic_model_coking (state_estimation_example_v2_MM)

```
93
94  # Calculate the pyrolytic coking contribution
95
96  FOR z := 0 TO 1 DO
97    reaction_rate_pyrolytic(z) {kg/m2/s} * 1E3 {g/kg} =
98      #limit the reduction in diameter to prevent the model from failing due to pressure runaway
99      0.5 * (1 - TANH( 5 * (percentage_reduction_diam(z) - percentage_reduction_diam_maximum)/2))
100     * (
101     # For first reaction conrrsidered in the model
102       10^log_10_kinetic_constant_ref_temp('c1') {g coke/(m2.s)/(mol/m3)}
103     * EXP(-activation_energy('c1') {J/mol} / up.gas_constant {J/mol/K} * (1 / temperature(z) {K} - 1 / temperature_refere
104     * molar_concentration('propylene',z) {mol/m3}
105     # For second reaction considered in the model
106     + 10^log_10_kinetic_constant_ref_temp('c2') {g coke/(m2.s)/(mol/m3)}
107     * EXP(-activation_energy('c2') {J/mol} / up.gas_constant {J/mol/K} * (1 / temperature(z) {K} - 1 / temperature_refere
108     * (molar_concentration('ethylene',z) + 1E-9)^n_C2H4 {mol/m3}  {g/m2/s}
109     # For second reaction considered in the model
110     + 10^log_10_kinetic_constant_ref_temp('c3') {g coke/(m2.s)/(mol/m3)}
111     * EXP(-activation_energy('c3') {J/mol} / up.gas_constant {J/mol/K} * (1 / temperature(z) {K} - 1 / temperature_refere
112     * molar_concentration('1,3-BUTADIENE',z) {mol/m3}
113     # This term is based on the model proposed by Plehiers et al (1990)
114     + 10^log_10_kinetic_constant_ref_temp('c4')
115     * EXP(-activation_energy('c4') {J/mol} / up.gas_constant {J/mol/K} * (1 / temperature(z) {K} - 1 / temperature_refere
116     * molar_concentration('ethylene',z)^2
117     / (molar_concentration('propylene',z) + 1E-9)); {g/m2/s}
118
119 END # FOR z := 0 TO 1 DO
120
```

1:1 INS

Interface | Interface language | Topology | gPROMS language | Properties

Pressure drop equation:

$$A(z)\frac{\partial p(z)}{\partial z} = F(z)\frac{\partial v(z)}{\partial z} - A(z)\rho(z)v(z)\left[\frac{2}{R_I(z)}f_{tube}(z) + \frac{NB}{L}f_{bend}(z)\right],$$

$$@z = L: \quad p(z) = p^{outlet}$$

With

$$\frac{1}{\sqrt{4\left(\frac{f_{tube}}{f_{adjustment}}\right)}} = -2\log\left[\frac{\frac{K(z)}{d_i}}{3.71} + \left(\frac{7}{Re}\right)^{0.9}\right],$$

$$K(z) = K_{clean\ tube} + \alpha r_{coking}(z)$$

$$f_{bend}(z)\left(0.7 + \frac{\alpha}{90}0.35\right)(0.051 + 0.19\frac{2R_I(z)}{R_B})$$

gCRACKER v. 1.0: Furnace Model

Heat transfer model

$$q_{ext}(z)R_0 = U(z)R_I(z)[T_I(z) - T_G(z)] = \\ = \frac{\lambda_c[T_W(z) - T_I(z)]}{\ln\left(\frac{R_W}{R_I(z)}\right)} = \frac{\lambda_w[T_0(z) - T_W(z)]}{\ln\left(\frac{R_0}{R_W}\right)}$$

R_0= external radius
R_w= internal radius of the tube
$R_I(z)$ = radius at interface coke-gas
Temperatures accordingly

$$U(z) = \frac{Nu(z)\lambda_G(z)}{2R_I(z)}$$

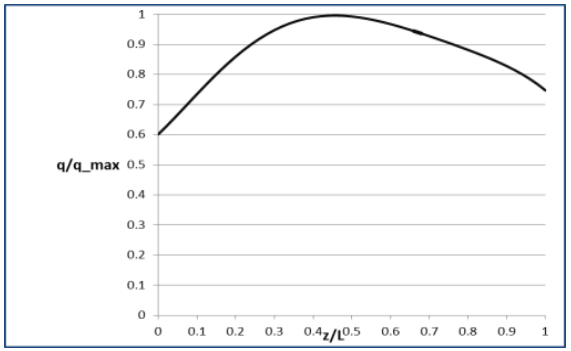
with

$$Nu(z) = 2.43E-02 Re(z)^{0.8}\,\mathrm{Pr}(z)^{0.4} + \frac{429.2}{l(z)^{0.0706}} - \frac{544.3}{\left(\frac{X(z)}{100}\right)^{0.0437}}$$

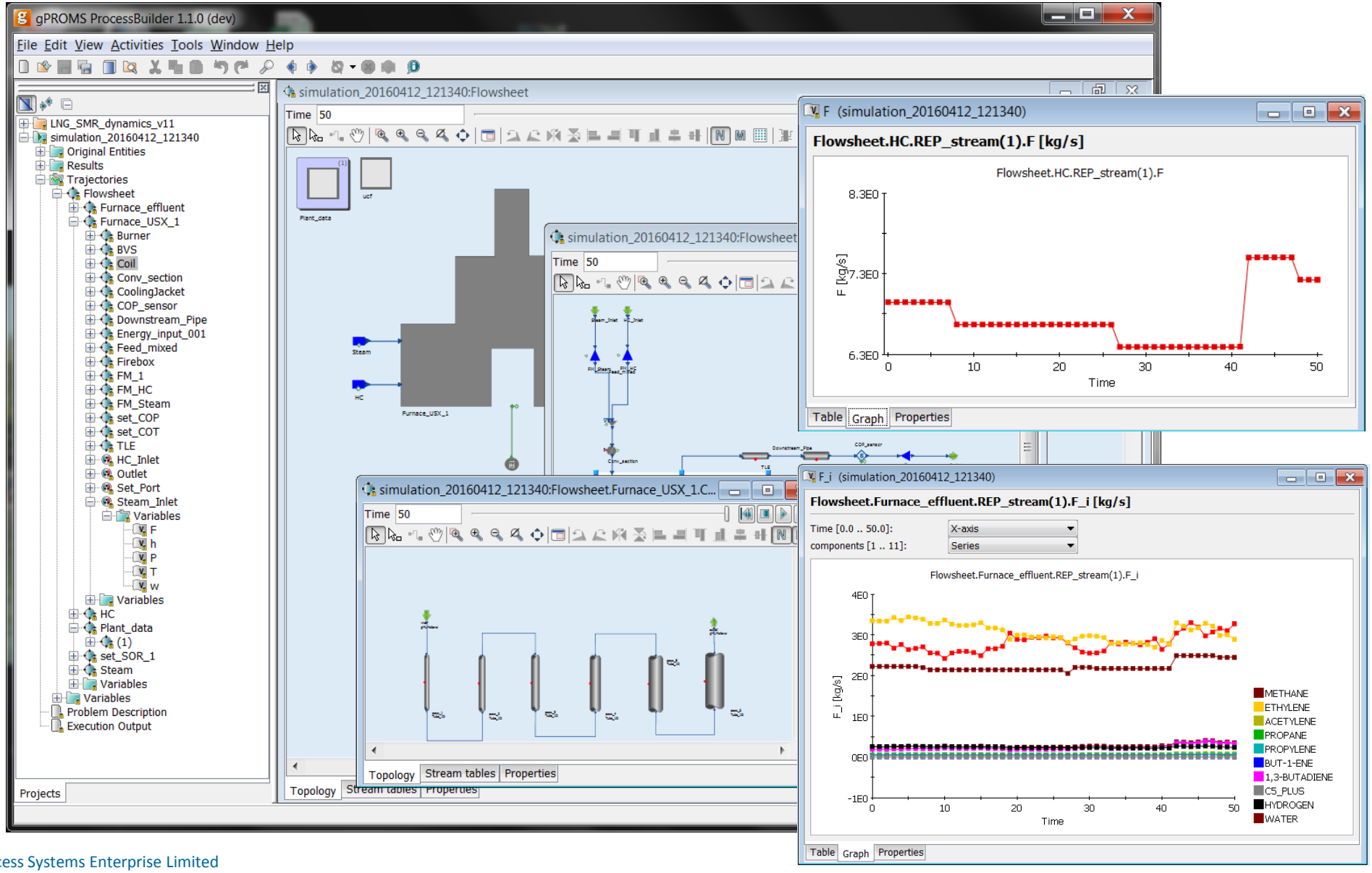
and

$$l(z) = \frac{2z}{Re(z)\,\mathrm{Pr}(z)R_I(z)}$$

- An external *a priori* heat flux profile $q_{ext}(z)$ is assigned :



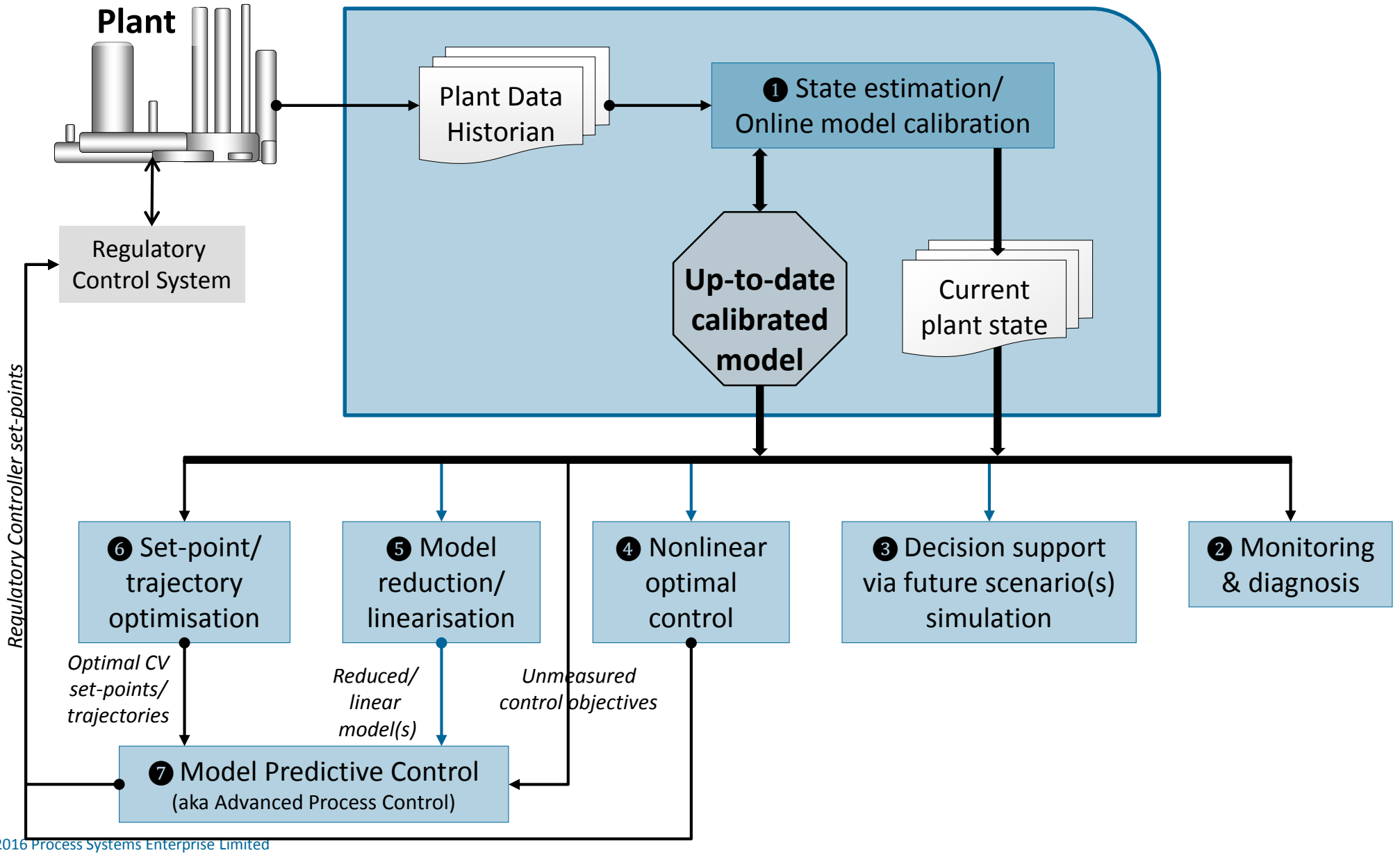
Execute simulation



Online Model-based Application (OMBA)

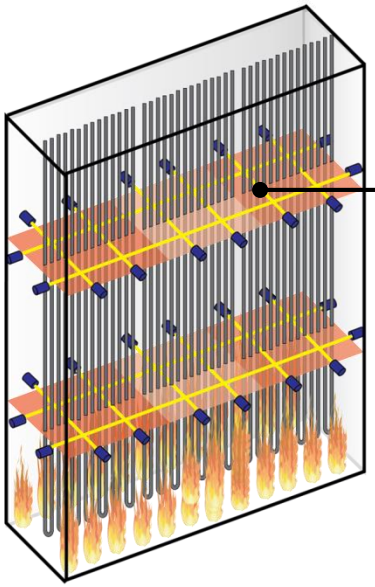
Online Model-Based Applications (OMBAs)

Integrated framework – the 'big picture'



gCRACKER Online v1.0 approach

Parallel model execution



Cracking furnace radiant cell

Plant Data Historian

gCRACKER Online

❶ Parallel model execution based on plant data

Product yields, key temperatures other KPIs

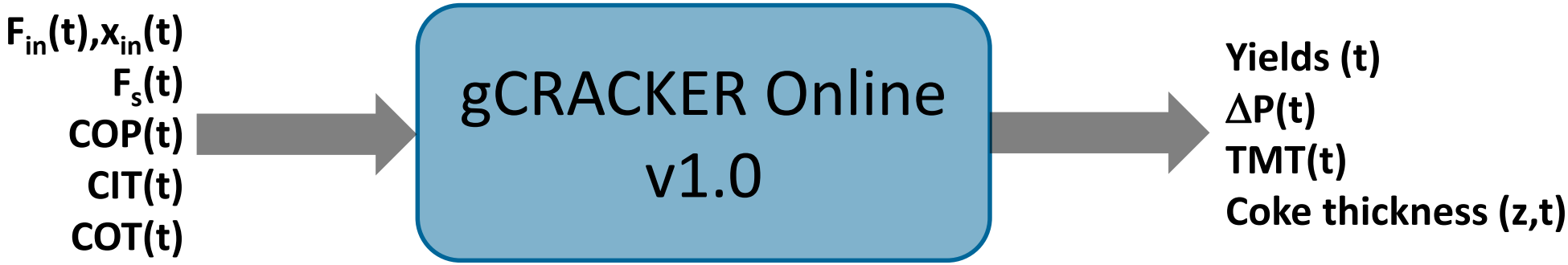
Current state of coking

❹ Olefin plant optimisation

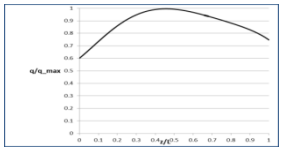
❸ Cracking furnace control & operations decision support

❷ Monitoring & diagnosis

gCRACKER Online v1.0



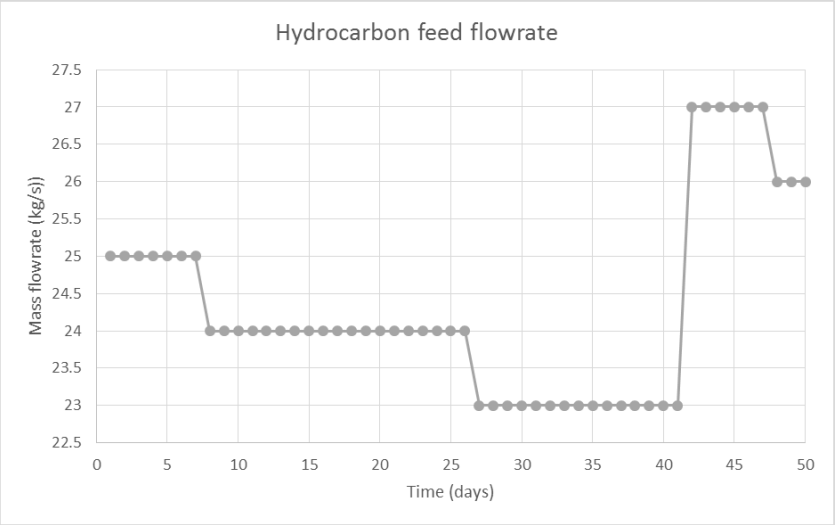
- **Uses gCRACKER model of furnace operation**
  - ethane/propane/mixed feeds
  - given shape of axial heat flux profile

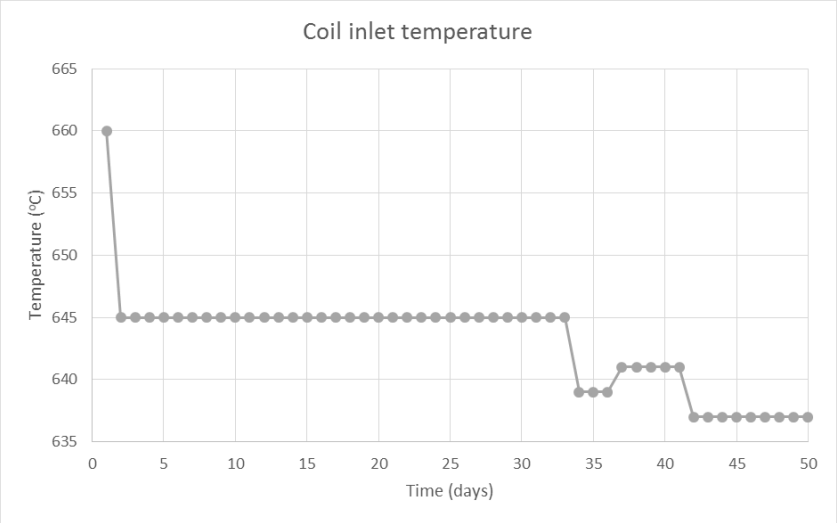


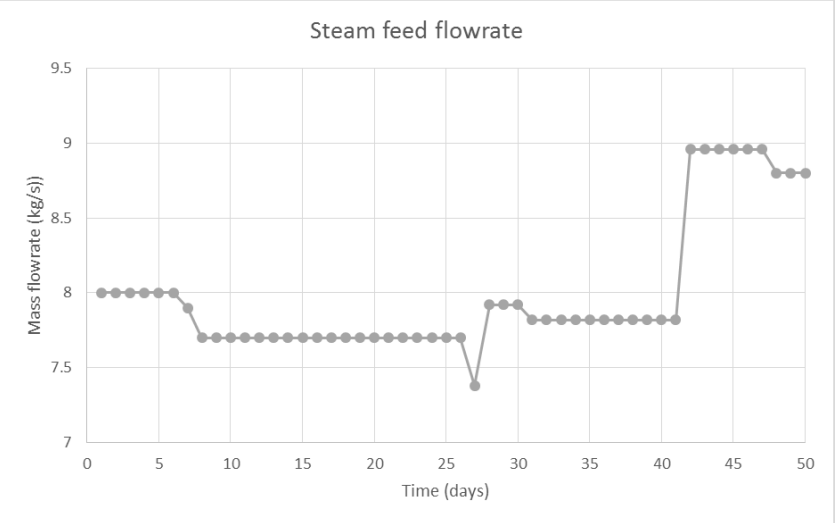
- **A dynamic simulation-based calculation based on quasi-steady-state model**
  - all inputs are specified degrees of freedom in the model
  - all outputs are computed model variables
  - execution much faster than real time
- **Successfully deployed online within DCS**
  - 8 furnaces × 2 cells
  - 16 gO:RUNs executing simultaneously in real time

gCRACKER Online v1.0
Trial

- Run of 50 days
- Changing feedstock rates, inlet temp, dilution steam
- Predict using proposed coking kinetics
- Compare outputs with plant data

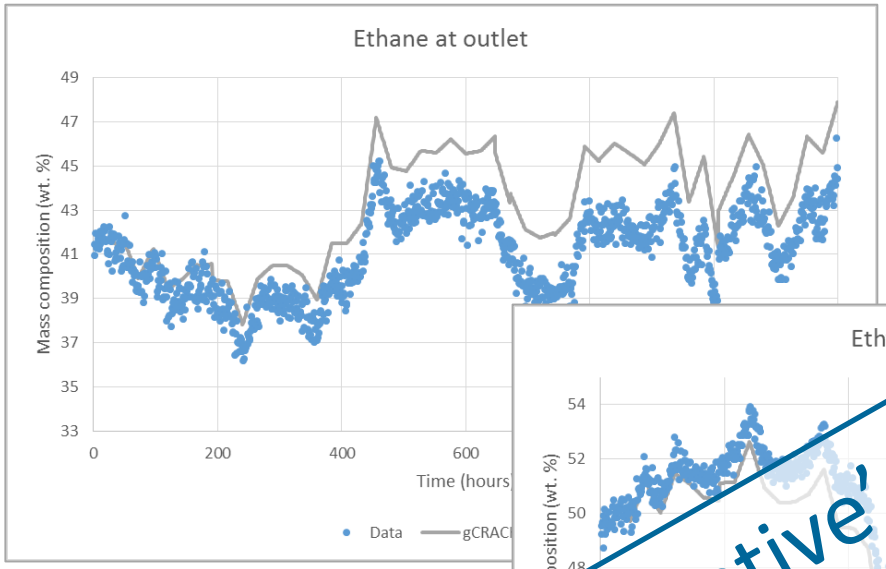


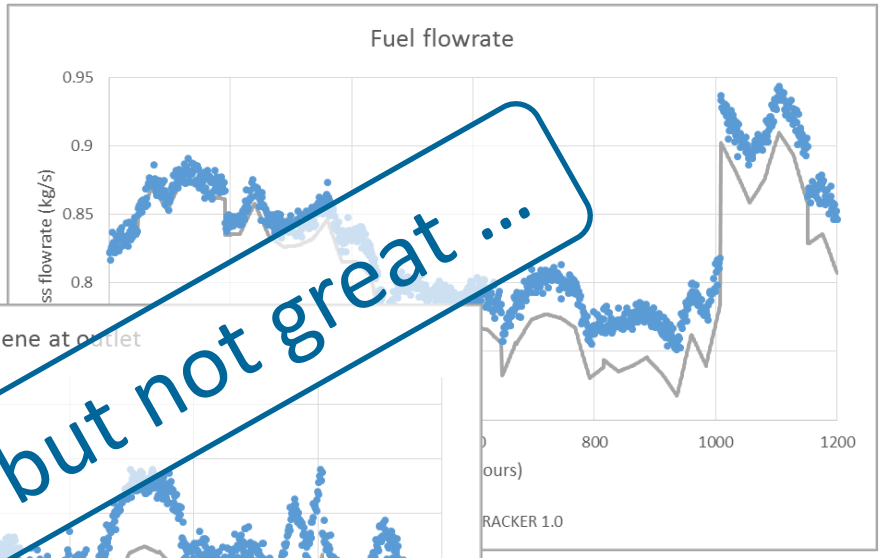


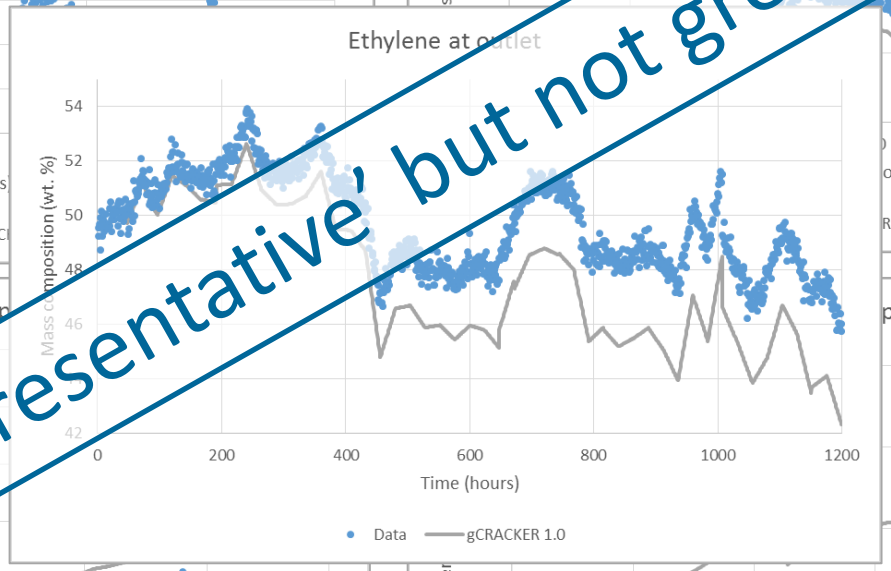


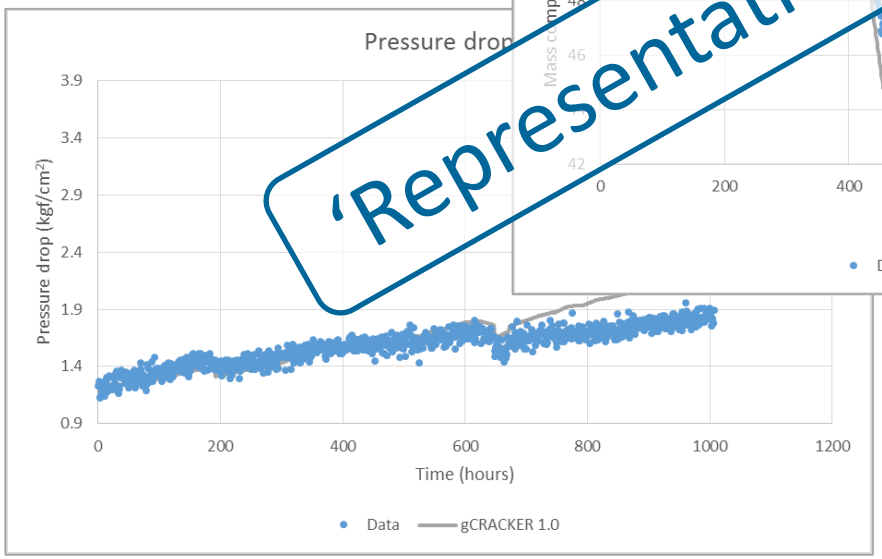
gCRACKER Online v1.0

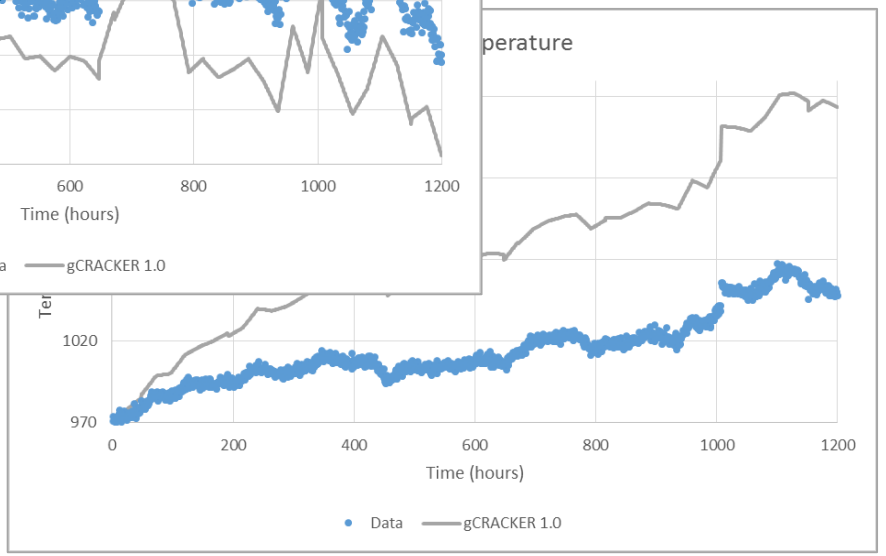
Results 1





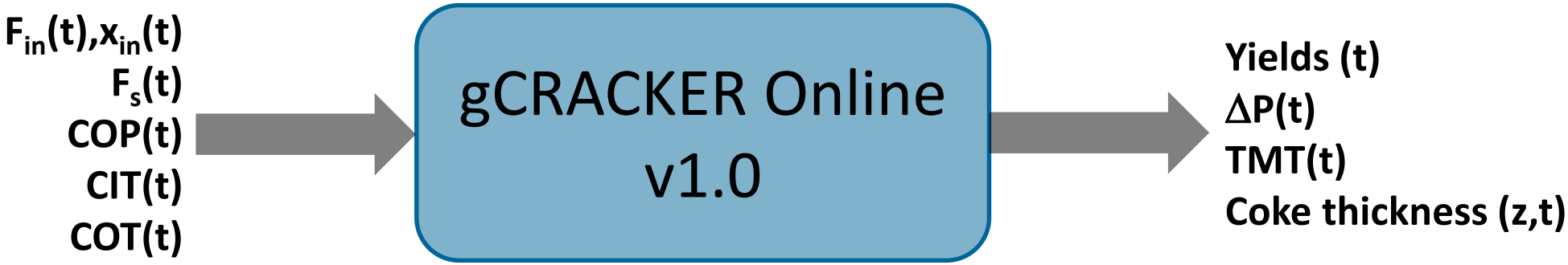






'Representative' but not great ...

gCRACKER Online v1.0



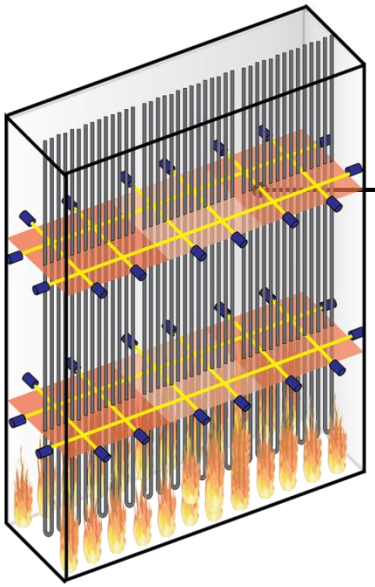
Why?

- **Some of the inputs may not be accurate**
  - e.g. COT not measured directly
- **Model is subject to inaccuracies**
  - characterisation of coking ➔ prediction of coke thickness
  - heat losses ➔ relation between conversion & fuel consumption?
- **What if we have some additional ("redundant") measurements relating to model <u>outputs</u>?**

CAN WE DO BETTER?

gCRACKER Online v2.0 approach

State estimation



Cracking furnace radiant cell

Plant Data Historian

gCRACKER Online

❶ State estimation/ Online model calibration

Up-to-date calibrated model

Product yields, key temperatures other KPIs

Current state of coking

❹ Olefin plant optimisation

❸ Cracking furnace control & operations decision support

❷ Monitoring & diagnosis

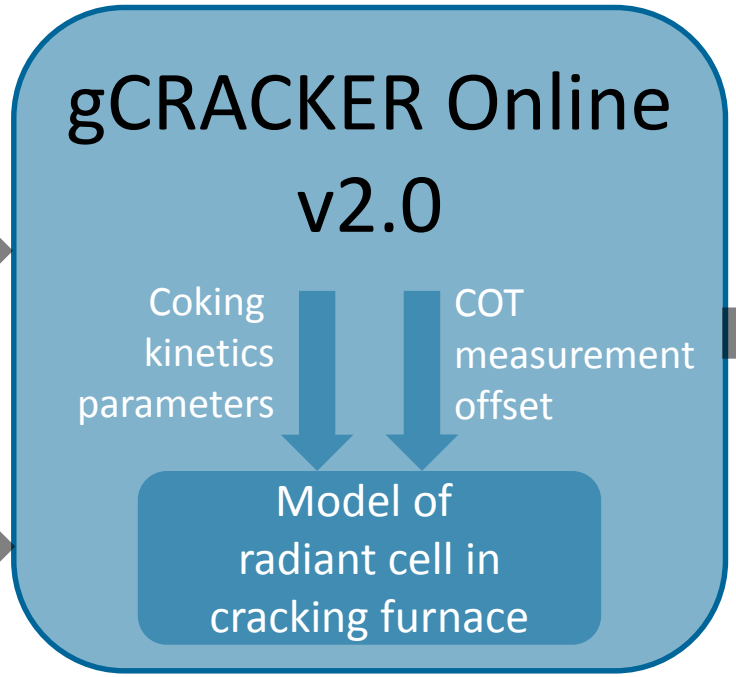
CVs, MVs and KPI outputs

Control inputs
(no/little uncertainty)

$F_{in}(t), x_{in}(t)$
$F_s(t)$
COP(t)
CIT(t)

Plant measurements
(uncertainty in measurements)

$\widehat{\Delta P}(t)$
$CST(t)$
$TMT(t)$
$\hat{x}^{out}_{ethylene}(t)$
$\hat{x}^{out}_{ethane}(t)$



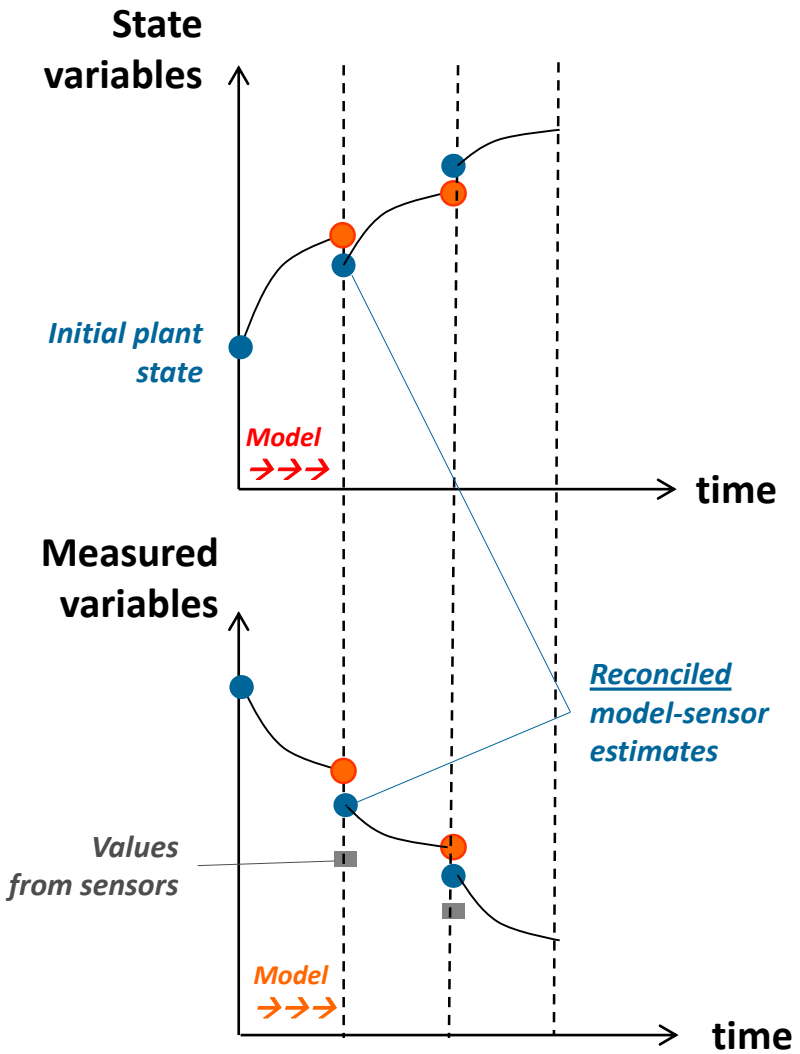
Optimal KPI estimates

Yields (t)
$\Delta P(t)$
TMT(t)
Coke thickness (z,t)
COT(t)
Fuel Consumption (t)

- **Model-based state estimation**
  - makes use of any available redundant measurements
  - takes account of uncertainty in both measurements and model
- **Continuously self-calibrating model**
  - coking kinetics
  - furnace heat losses
  - . . . . . …

- Apply physical understanding to identify weak points of model
- Focus state estimation specifically on these points

State Estimation
for Online Model-Based Applications



- Reconcile
  - model predictions
  - sensor measurements
- to obtain a better estimate of the current state of the system
  - process variables
    - compositions, temperatures, pressures, flowrates, ….
  - plant characteristics that may gradually change during operation
    - catalyst activity
    - heat transfer coefficients
    - rotating equipment performance parameters
- …and of the uncertainty in these estimates

State Estimation
Extended Kalman Filter

- Extended Kalman Filter (EKF) algorithm chosen
  - EKF is well-established and implementation is relatively simple
  - Investigating other options too

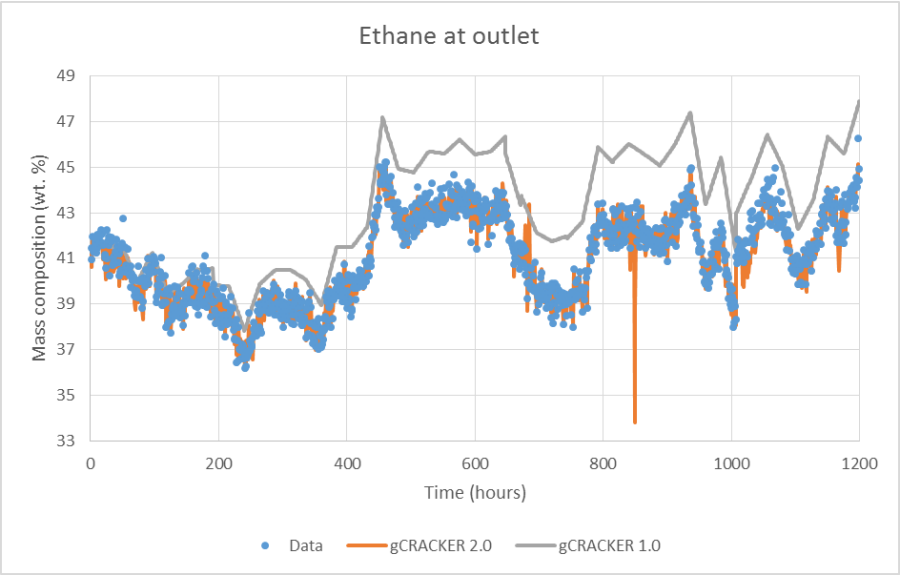
- Prototyped on large-scale client application

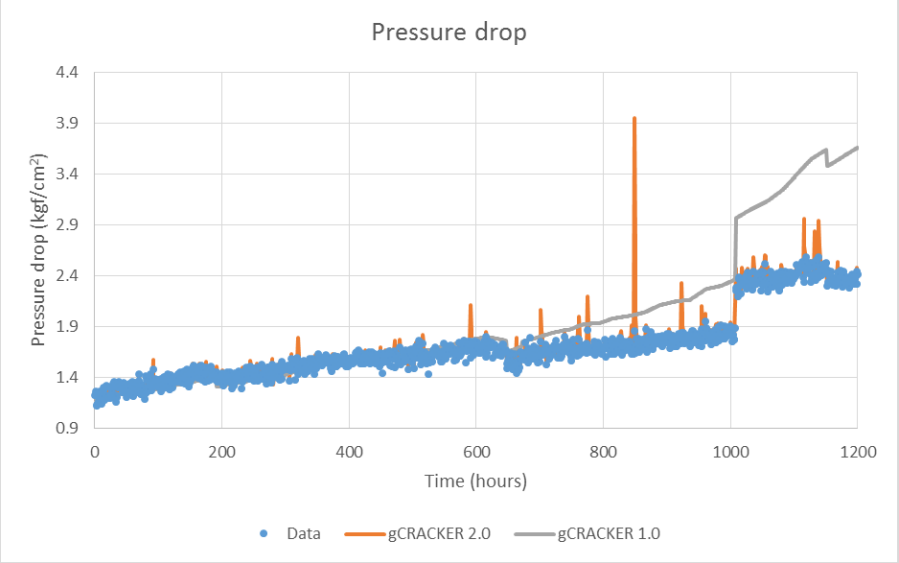
➔ Now being formally implemented within gPROMS online toolkit using DAEBDF integrator

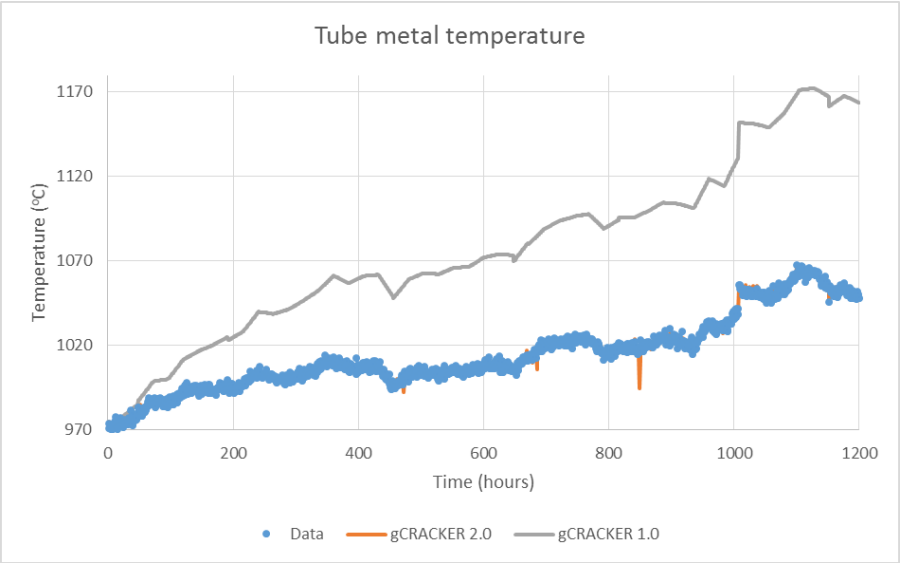
gCRACKER Online v2.0

Results 1

- Run against same plant data, but use state estimation to:
  - adjust state variables
  - adjust coking kinetics
  - adjust COT offset
  - …







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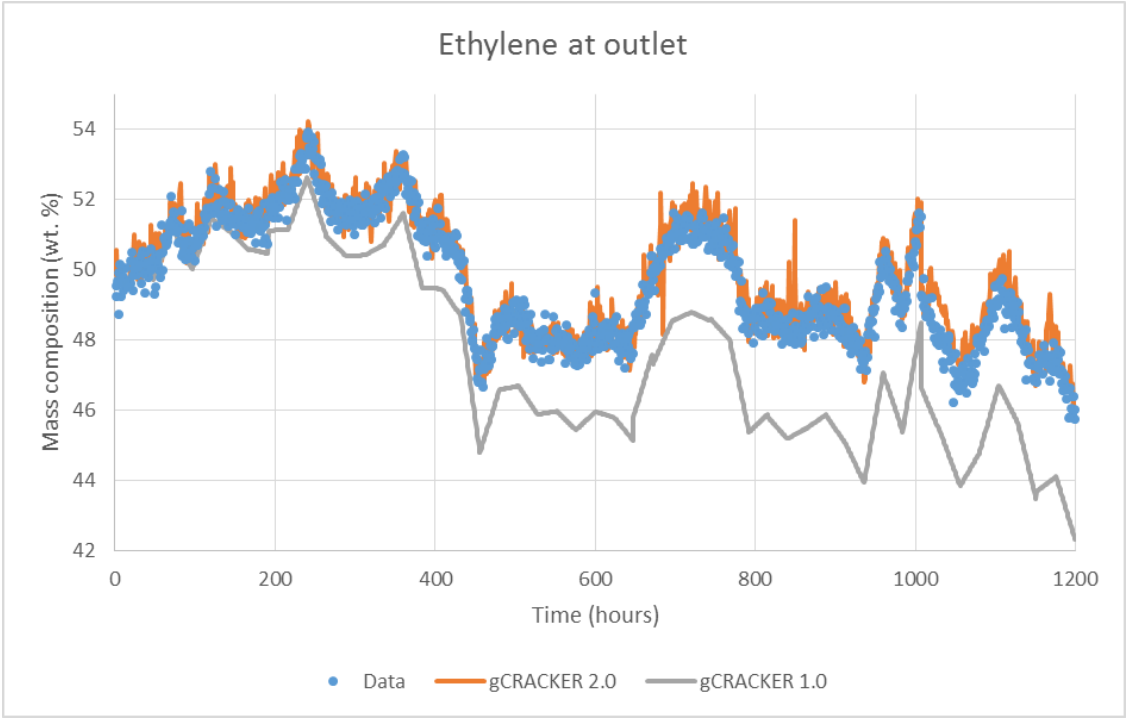
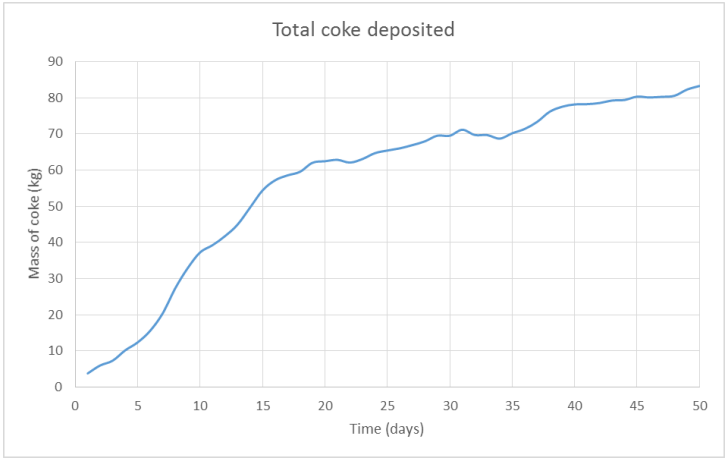
Results 2

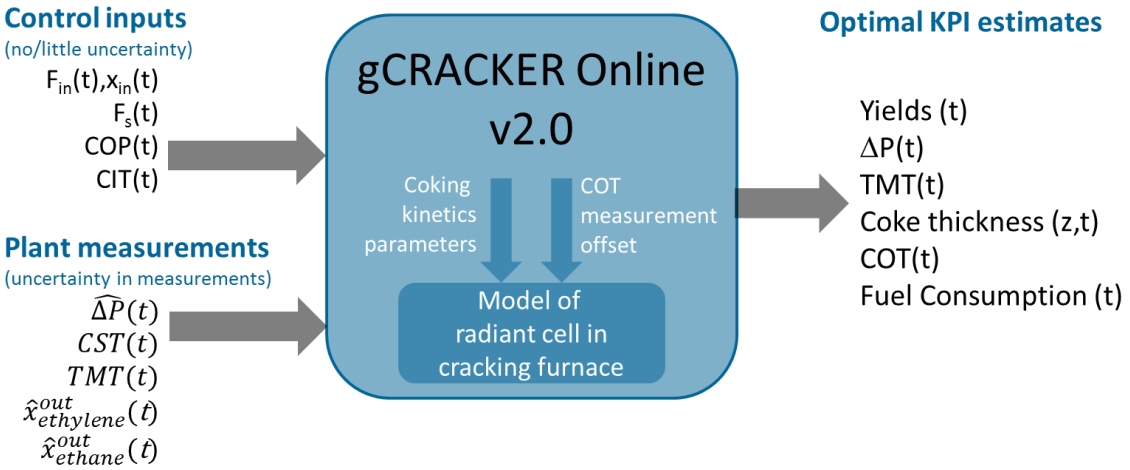
- Key result: Ethylene *estimate*
- Plant measurements NOT made available to gCRACKER





< Cumulative coke deposit also useful to know

Conclusions



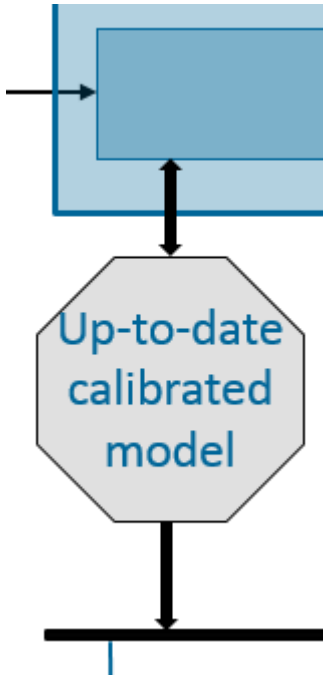
Mathematical structure

- ✓ PDAE system
- ✓ 200+ differential equations
- ✓ ~15000 algebraic equations

1 – 2 hours for 50 days

Key information generated for each cell in each furnace

1. **Reliable estimate of current state of coking**
   - significant effect on optimal solution
2. **Accurate KPI and other variable information**
3. **Up-to-date model**
   - ➔ use in whole-plant optimisation application
   - ➔ possibility for more sophisticated control



➔ **Can be applied to many other processes**

Thank you