Interval based dynamic simulations in chemical process design

By

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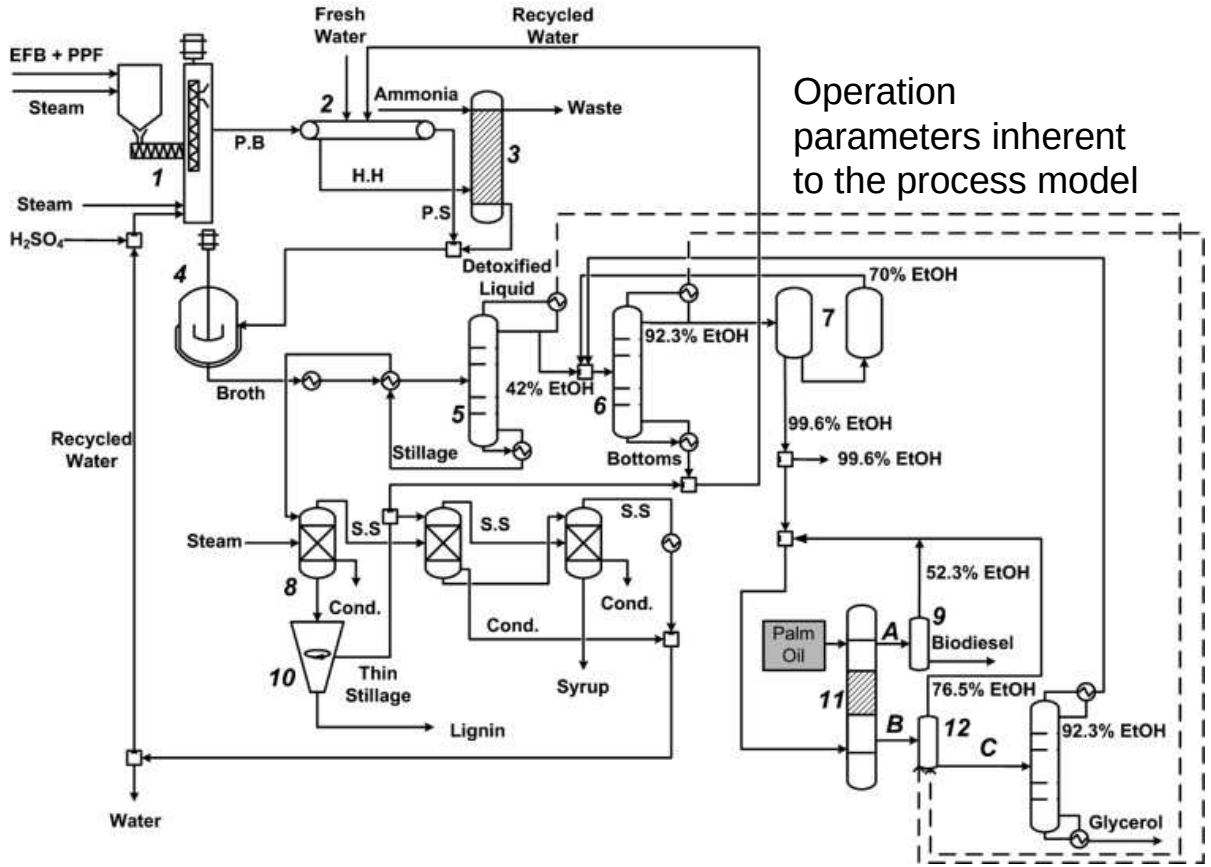
Outline

- CHEMICAL PROCESS DESIGN
- PROBLEMS ARISING IN CHEMICAL PROCESS DESIGN
- INTERVAL BASED DYNAMIC SIMULATIONS
- MATHEMATICAL DESCRIPTION OF THE PROBLEM
- INTERVAL INITIAL VALUE PROBLEM SOLVERS USED
- CASE STUDIES
- CONCLUSIONS
- FUTURE WORK
- ACKNOWLEDGEMENTS

Chemical process design

Chemical process design is concerned with establishing equipment parameters and operating conditions for the structure of the process.

Initial conditions t=0



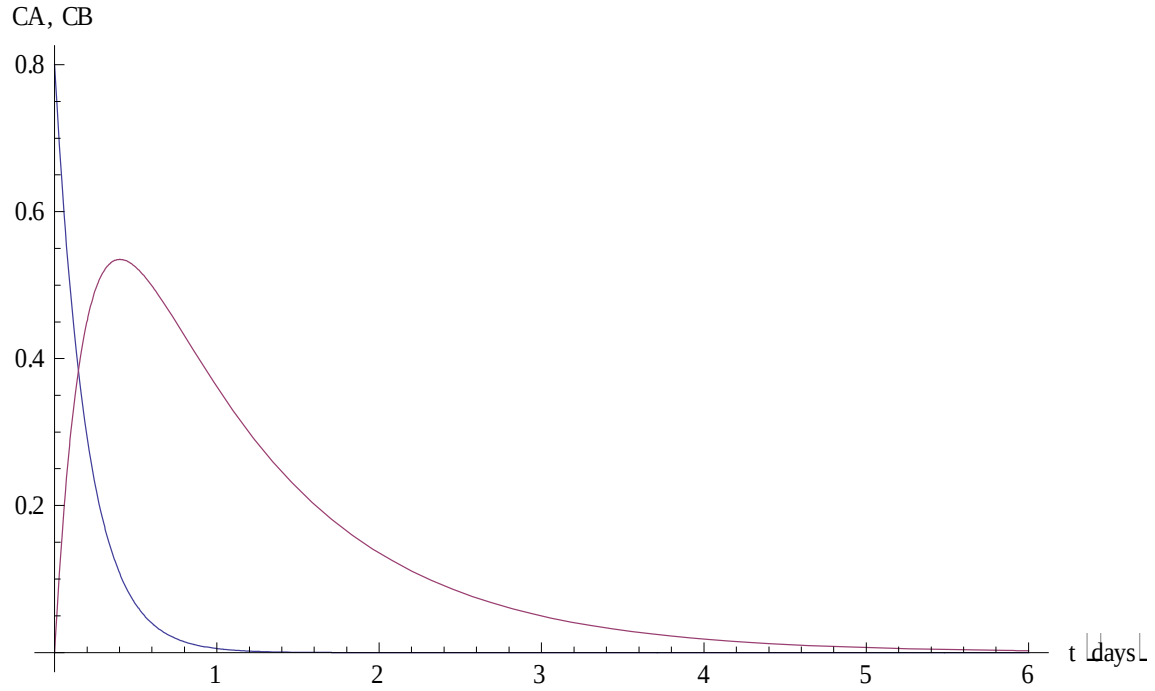
Operation parameters inherent to the process model

PARTICULAR DESIRED OUTCOME (AMOUNT, QUALITY)

Chemical process design (continued)

Dynamic simulation is a useful tool for chemical process design as it give us valuable information to determine what actions should be taken to achieve the desired outcome.

$$\mathrm{CA}'(t) = -k_1 * \mathrm{CA}(t)$$
$$\mathrm{CB}'(t) = k_1 * \mathrm{CA} - k_2 * \mathrm{CB}$$
$$t_0 = 0, \mathrm{CA}(t_0) = 0.8, \mathrm{CB}(t_0) = 0, k_1 = 5\mathrm{day}^{-1}, k_2 = 1\mathrm{day}^{-1}$$



Problems arising in chemical process design

- When uncertain parameters or initial conditions arise in dynamic process models it becomes challenging to rigorously obtain the output.
- Ordinary numerical solvers can fail.
- Guaranteeing bounded performance across the whole trajectory of complex chemical systems remains a challenge.

$$\mathrm{CA}'(t) = -k_1 * \mathrm{CA}(t)$$
$$\mathrm{CB}'(t) = k_1 * \mathrm{CA} - k_2 * \mathrm{CB}$$

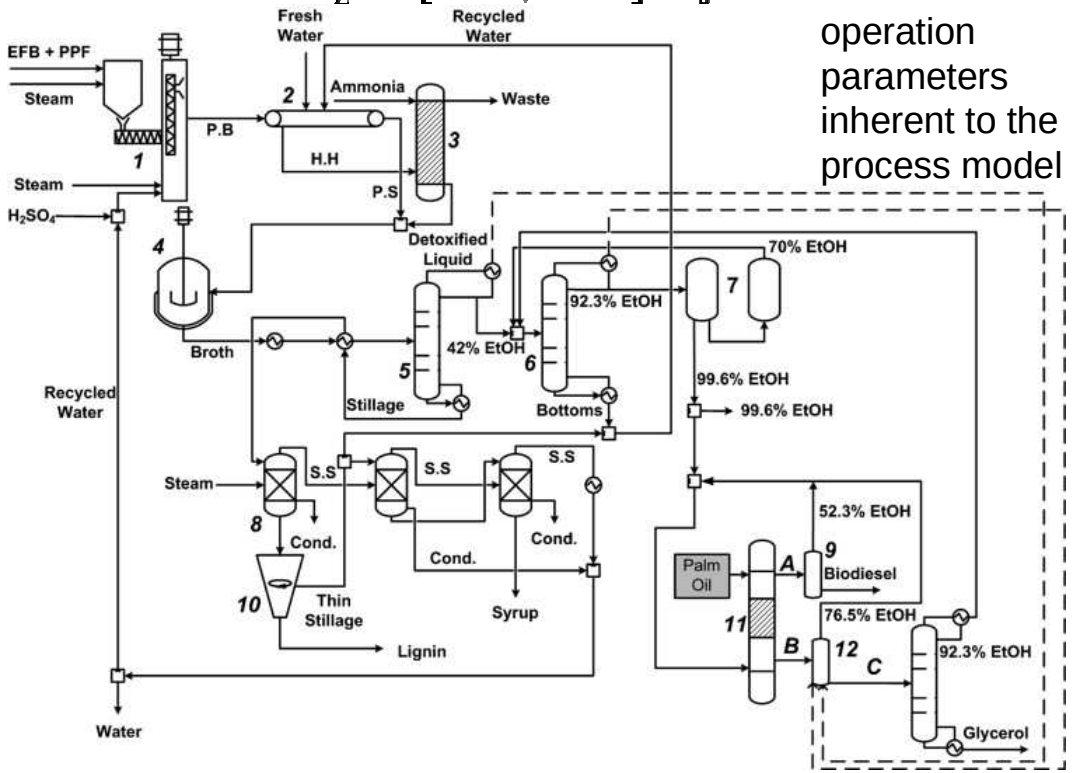
Initial conditions

$$t_0 = 0$$
$$\mathrm{CA}(t_0) = [0.7, 0.9]$$
$$\mathrm{CB}(t_0) = 0$$

Parameters

$$k_1 = [4.5, 5.5]\mathrm{day}^{-1}$$
$$k_2 = [0.95, 1.05]\mathrm{day}^{-1}$$

Uncertain initial conditions t=0

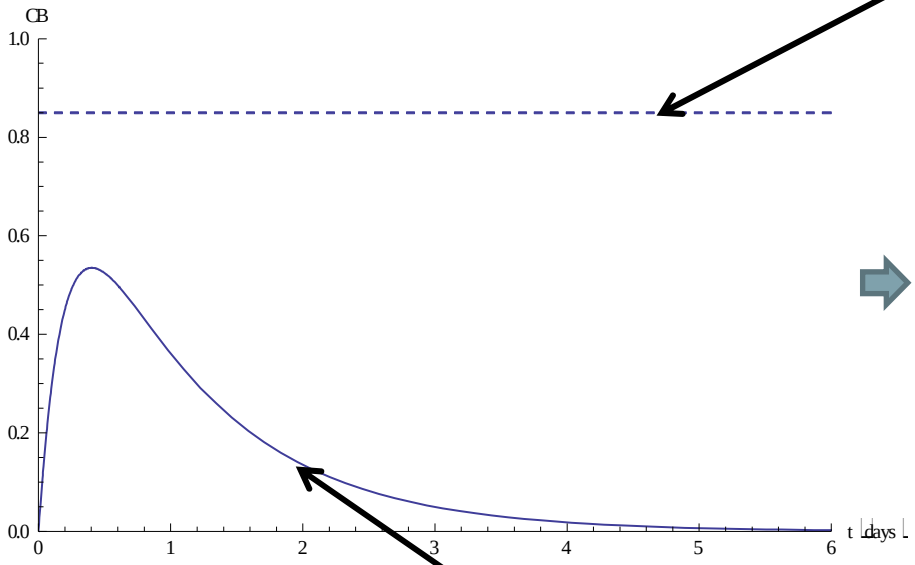


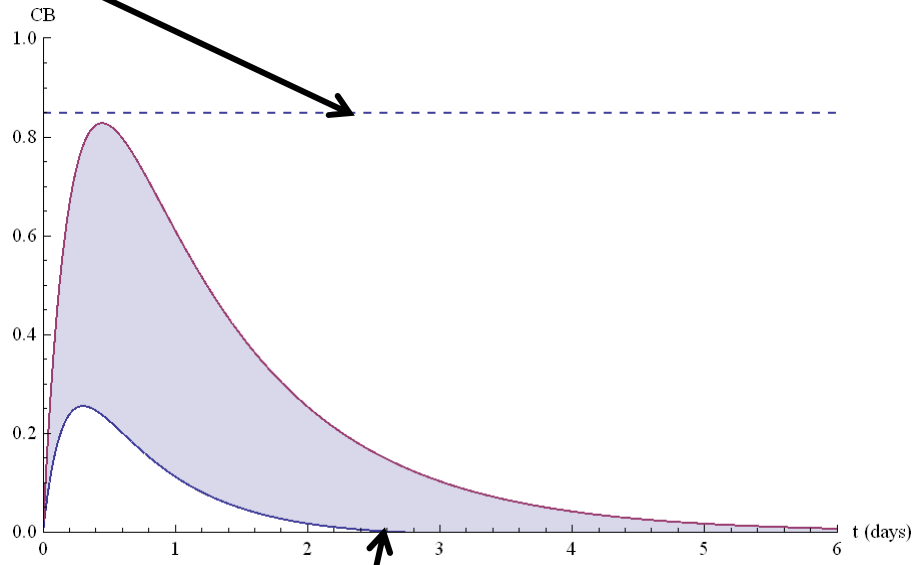
Uncertain operation parameters inherent to the process model

UNCERTAIN OUTCOME WHERE THE PARTICULAR DESIRED OUTCOME MAY LIE (AMOUNT, QUALITY)

Interval based dynamic simulations

Safety constraint that the process must meet





Optimal performance for a given process

Bounded performance taking into account uncertainty

Mathematical description of the problem

Mathematical problem

$$y'(t) = f(y),$$
$$y(t_0) = [y_0]$$

Reformulation into integral equation

$$Py(t) = y_j + \int_{t_j}^{t} f(y(s))ds$$

Taylor series

$$[y(t)] = [y_j] + \sum_{i=1}^{k-1} f^i([y_j])(t - t_j)^i + f^k([\tilde{y}_j])(t - t_j)^k$$

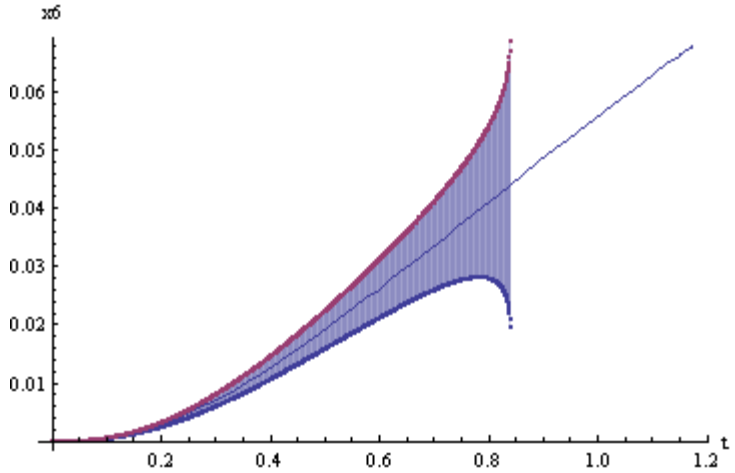
$$[y_{j+1}] = [y_j] + \sum_{i=1}^{k-1} f^i([y_j])h_j^i + f^k([\tilde{y}_j])h_j^k$$

Mathematical description of the problem (continued)

Mean-value evaluation

$$[y_{j+1}] = \hat{y}_j + \sum_{i=1}^{k-1} f^i(\hat{y}_j)h_j^i + f^k([\tilde{y}_j])h_j^k + \left\{ I + \sum_{i=1}^{k-1} J(f^i;[y_j])h_j^i \right\}([y_j] - \hat{y}_j)$$

The methods used are mainly focused on how to reduce the wrapping effect



Interval initial value problem solvers used

- The methods that have been used were developed by Moore, Eijenraam and Lohner.
- They are focused on giving a solution for the reformulated initial value problem
- Different reformulation to avoid wrapping effect.

Interval initial value problem solvers used (continued)

- Chemical engineering test problems were solved with an initial value problem solver.
- Uncertainty was taken into account
- A disturbance was generated at time *t* in the model

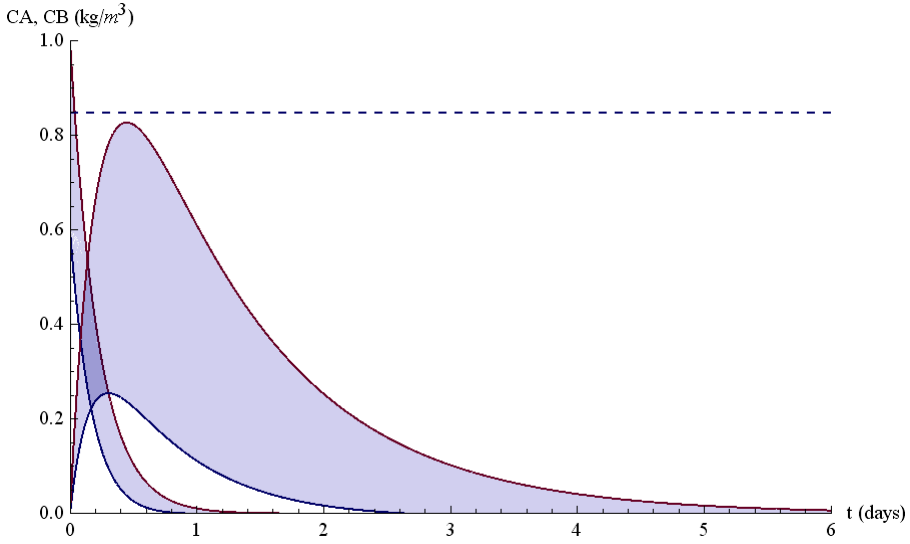
Case studies

- First order reactor

$$\frac{dC_A}{dt} = -k_1 C_A$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$$

$$k_1 = [4.5, 5.5]\text{day}^{-1}$$
$$k_2 = [0.95, 1.05]\text{day}^{-1}$$



Simulation of first order reactor with uncertain parameters

Case studies

- Bioreactor

$$\frac{dX}{dt} = (\mu - \alpha D)X$$

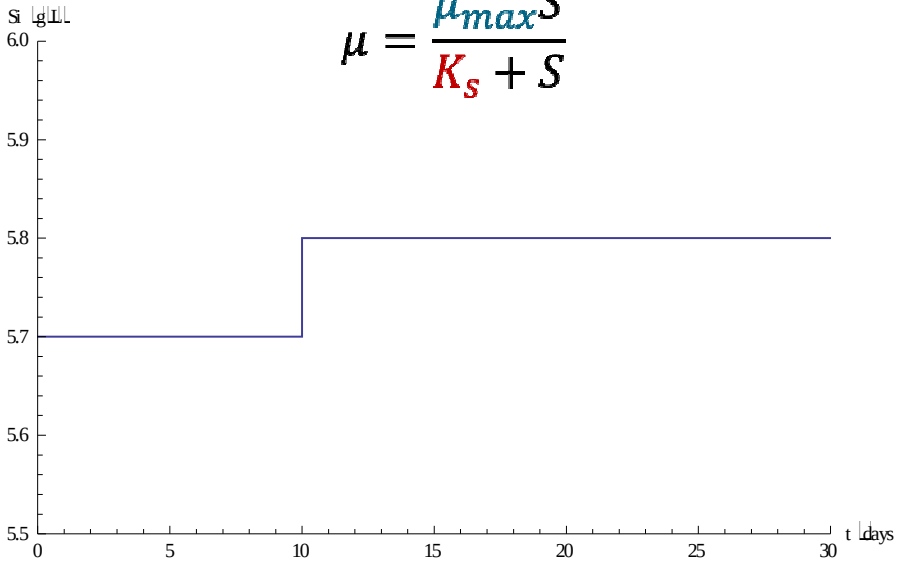
$$\frac{dS}{dt} = D(S_i - S) - k\mu X$$

$$\mu = \frac{\mu_{max} S}{K_s + S}$$

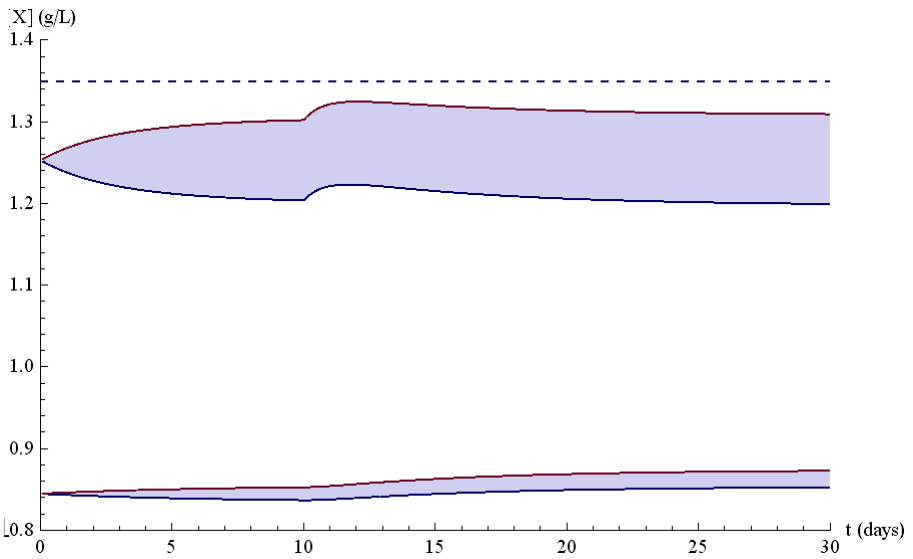
Interval parameters

$K_s = [7.09, 7.11]\ g/L$

$\mu_{max} = [1.19, 1.21]\ day^{-1}$



Disturbance generated at *t*=10 days



Simulation of the process with uncertain parameters

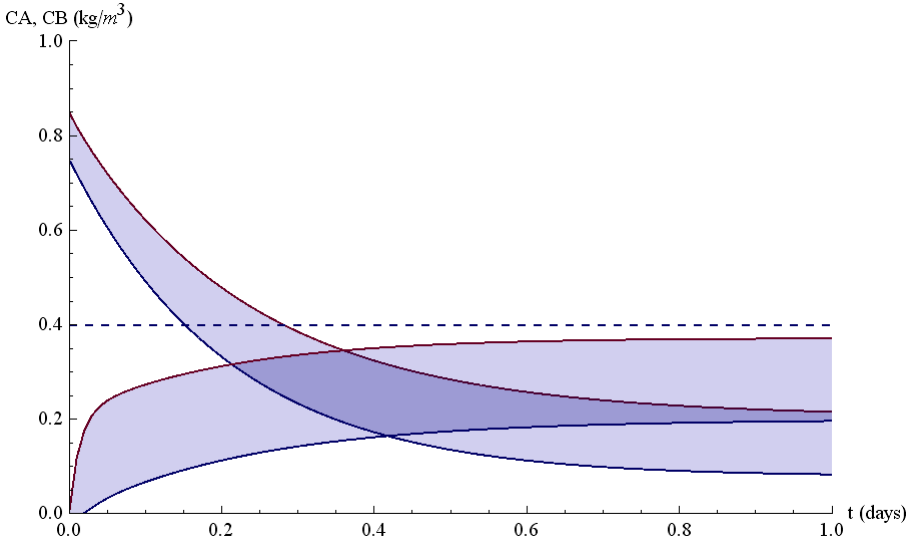
Case studies

- First order reversible reactor

$$\frac{dC_A}{dt} = -k_1 C_A - k_{-1} C_B$$

$$\frac{dC_B}{dt} = k_1 C_A - (k_{-1} + k_2) C_B + k_{-2}(1 - C_A - C_B)$$

$$k_1 = [3.8, 4.2]\text{day}^{-1}$$
$$k_{-2} = [18, 22]\text{day}^{-1}$$
$$C_A(0) = [0.75, 0.85]\text{kg/m}^3$$



Simulation of first order reactor with uncertain parameters

Case studies

- Glucagon receptor model

$$\frac{dR_r}{dt} = k_{-1}LR_u - L(t)k_1R_r - k_sR_r + k_rR_s$$

$$\frac{dR_s}{dt} = k_{sp}LR_p + G_iK_{2s}LR_u + k_s(LR_u + R_r) - k_rR_s$$

$$\frac{dG_i}{dt} = -G_iK_{23}LR_u + G_*\left(k_h + \frac{Ca(t)k_{Gdeg,Cal}}{K_{Gdeg,Cal} + G_*} + \frac{PLC_*k_{Gdeg,PLC}}{K_{Gdeg,PLC} + G_*}\right)$$

$$G_* = G_0 - G_i$$

$$\frac{dLR_p}{dt} = -k_{sp}LR_p + k_p\left(1 + \frac{A_0}{1 + B_1{G_*}^{-n_1}}\right)\left(\frac{LR_u}{LR_u + B_2}\right)$$

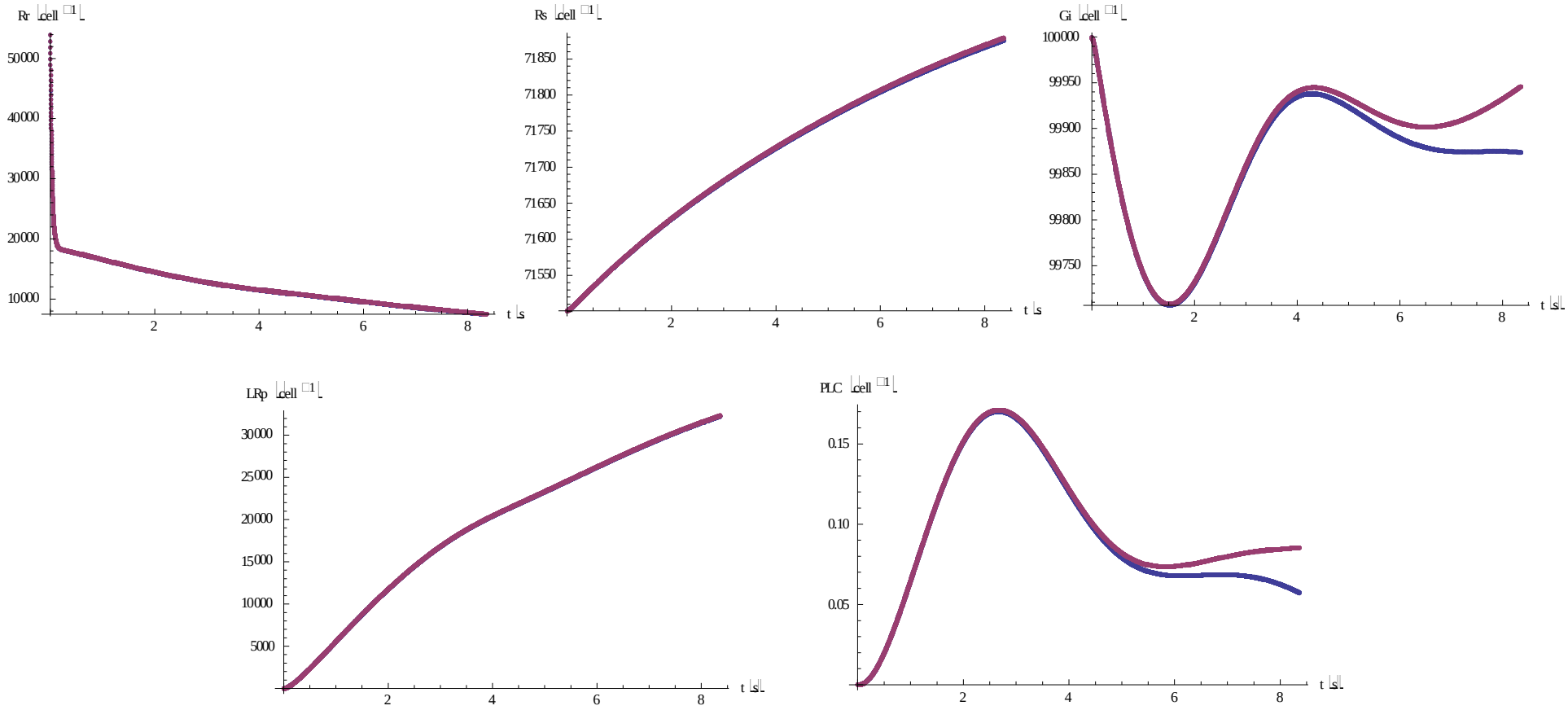
$$R_0 = R_r + R_s + LR_u + LR_p$$

$$\frac{dPLC_*}{dt} = k_{PC}G_* - \frac{PLC_*k_{PC,deg}}{K_{PC,deg} + PLC_*}$$

$$R_0 = [126475,126525]\text{cell}^{-1}$$

Case studies

- Glucagon receptor model (continued)



Simulation of the glucagon receptor model with an uncertain parameter

Case studies

- Reactor-separator model

$$\frac{dx_1}{dt} = \frac{F+B}{H}(x_F - x_1) + kx_1(1-x_1)$$

$$x_F = \frac{Fx_{F0} + Bx_2}{F+B}$$

$$y_i = \frac{\alpha x_i}{1+(\alpha-1)x_1}$$

$$\frac{dx_2}{dt} = (L+F+B)x_3 - Bx_2 - Vy_2$$

$$\frac{dx_3}{dt} = (L+F+B)(x_4 - x_3) + V(y_2 - y_3)$$

$$\frac{dx_4}{dt} = (F+B)x_1 + Lx_5 - (L+F+B)x_4$$

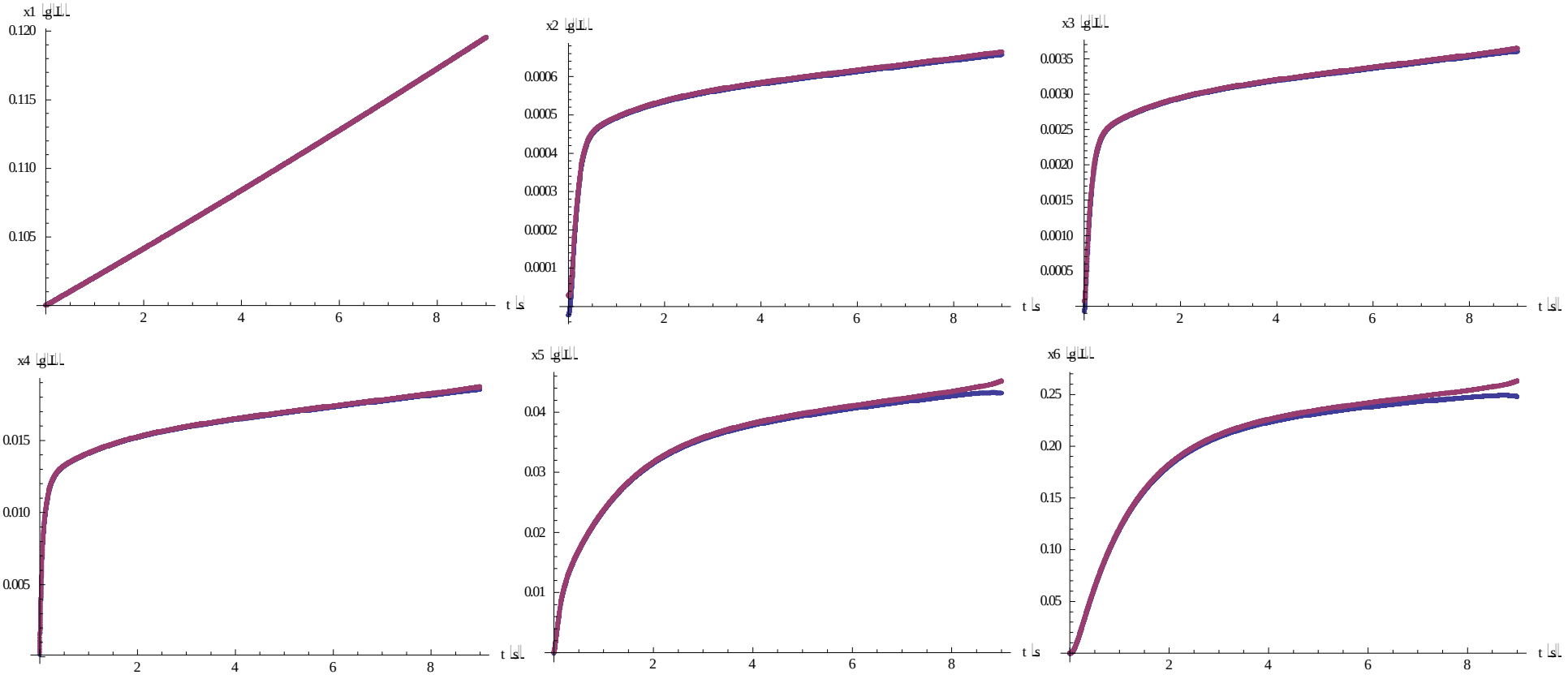
$$\frac{dx_5}{dt} = L(x_6 - x_5) + V(y_4 - y_3)$$

$$\frac{dx_6}{dt} = -(L+D)x_6 + Vy_5$$

$L = [1.703, 1.705] \mathrm{kg/m^3}$

Case studies

- Reactor separator model (continued)



Simulation of the reactor separator model with an uncertain parameter

Conclusions

- Interval methods are very useful to obtain the bounded performance of chemical processes of interest.
- Obtaining bounds for more complex systems across the whole trajectory remains a challenge.

Future work

- Reformulation techniques to avoid the dependency problem.
- Implementation of QR factorization enclosure methods and Taylor Models.
- Increase the variety of Chemical Engineering problems, increase dimensionality and include events.
- Implementation of Global Optimisation algorithms to determine optimal robust trajectories.

Acknowledgements

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Thank you for your attention!