temperature independent, i.e., $\hat{H}_j^\circ$ is temperature independent, this requires that $\tilde{c}^\bullet_{p,\mathrm{B}} - a\tilde{c}^\bullet_{p,\mathrm{A}} \equiv 0$ — or $\tilde{c}^\bullet_{p,\mathrm{B}} \equiv \tilde{c}^\bullet_{p,\mathrm{A}}$. The parameters and operating conditions in Tables 3-4 of (Sund et al., 2018) are judiciously chosen to ensure that the solvent-dominating model is identical to the model in (Seborg et al., 2011).

B Model linearization

For the model, with $x = (T, c_A)$, $u = (T_\mathrm{c}, T_\mathrm{i}, \dot{V}_\mathrm{i}, c_{\mathrm{A,i}})$, and $y = T$, the linearized model is:

$$\frac{dx^\delta}{dt} = Ax^\delta + Bu^\delta \tag{38}$$

$$y^\delta = Cx^\delta + Du^\delta \tag{39}$$

where for any z, $z^\delta \triangleq z - z^*$ and asterisk $*$ indicates nominal value. Using the Python API described in (Lie et al., 2016) together with OpenModelica, let `sr_org` be a Python object of the original reactor in (Seborg et al., 2011) (but with n_A replacing c_A as state). We can then linearize the model in Python with the statement:

```
>>> A, B, C, D = sr_org.linearize()
```

The following system matrices are found:

$$A = \begin{pmatrix} 4.3796 & 209.205 \\ -0.035714 & -2 \end{pmatrix} \tag{40}$$

$$B = \begin{pmatrix} 2.09205 & 1 & 0 & 0 \\ 0 & 0 & 0.005 & 1 \end{pmatrix} \tag{41}$$

$$C = \begin{pmatrix} 1 & 0 \end{pmatrix} \tag{42}$$

$$D = \begin{pmatrix} 0 & 0 & 0 & 0 \end{pmatrix}. \tag{43}$$

The open loop eigenvalues of A are $\lambda = (2.83388381, -0.45432613)$, hence the system is open loop unstable. The open loop transfer function from T_c^δ to T^δ is

$$T^\delta(s) = 2.092 \frac{s+2}{s^2 - 2.38s - 1.288} \cdot T_\mathrm{c}^\delta(s) \tag{44}$$

which implies that the system has a "stable" zero at $s = -0.5$ at the nominal operating point.

C Extended LQ+I system

The extended LQ problem with integral action is given as follows. Thee extended system is[10]

$$\underbrace{\frac{d}{dt}\begin{pmatrix} x \\ z \end{pmatrix}}_{\tilde{x}} = \underbrace{\begin{pmatrix} A & 0 \\ C & 0 \end{pmatrix}}_{\tilde{A}} \tilde{x} + \underbrace{\begin{pmatrix} B \\ 0 \end{pmatrix}}_{\tilde{B}} u \tag{45}$$

while the extended cost function $\tilde{\mathscr{J}}$ given as

$$\tilde{\mathscr{J}} = \frac{1}{2}\int_0^\infty \left(e_{\tilde{x}}^T \tilde{Q} e_{\tilde{x}} + e_u^T R e_u\right) dt \tag{46}$$

where

$$\tilde{Q} = \begin{pmatrix} C^T Q_y C & 0 \\ 0 & Q_z \end{pmatrix}. \tag{47}$$

[10] T_ref acts as a disturbance

References

Brian D. O Anderson and John B. Moore. *Optimal Control: Linear Quadratic Methods*. Prentice-Hall, Inc., 1989.

Karl Johan Åstrøm and Richard M. Murray. *Feedback Systems. An Introduction for Scientists and Engineers*. Princeton University Press, Princeton, NJ, 2008. ISBN 978-0-691-13576-2.

Peter Fritzson. *Principles of Object-Oriented Modeling and Simulation with Modelica 3.3: A Cyber-Physical Approach*. Wiley-IEEE Press, Piscataway, NJ, second edition, 2015. ISBN 978-1-118-85912-4.

Michael A. Henson and Dale E. Seborg. *Nonlinear Process Control*. Prentice Hall, Upper Saddle River, New Jersey, 1997.

Huibert Kwakernaak and Raphael Sivan. *Linear Optimal Control Systems*. Wiley-Interscience, New York, 1972.

Bernt Lie, Sudeep Bajracharya, Alachew Mengist, Lena Buffoni, Arun Kumar, Martin Sjölund, Adeel Asghar, Adrian Pop, and Peter Fritzson. Api for accessing openmodelica models from python. In *Proceedings of EuroSim 2016*, Oulu, Finland, 2016, September 2016.

Jan M. Maciejowski. *Predictive Control with Constraints*. Prentice Hall, Harlow, England, 2002.

James B. Rawlings, David Q. Mayne, and Moritz M. Diehl. *Model Predictive Control: Theory, Computation, and Design*. Nob Hill Publishing, LLC, second edition, 2017.

Dale E. Seborg, Thomas F. Edgar, Duncan A. Mellichamp, and III Doyle, Frank J. *Process Dynamics and Control*. John Wiley & Sons, Hoboken, NJ, third edition edition, 2011. ISBN 978-0-470-12867-1. ISBN 978-0-470-12867-1.

Dan Simon. *Optimal State Estimation: Kalman, H Infinity, and Nonlinear Approaches*. Wiley-Interscience, Hoboken, New Jersey, 2006.

Sveinung M. Sund, Marianne Plouvier, and Bernt Lie. Comparison of simulation tools for dynamic models. In *Proceedings, SIMS 2018*, Oslo Metropolitan University, September 2018. SIMS, Linköping University Press.