

Modeling and Simulation of Distributed Systems

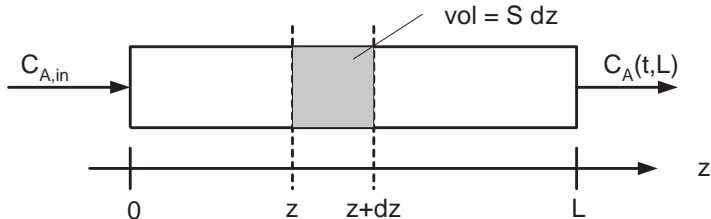
Partial Differential Equations

John Bagterp Jørgensen

*Department of Applied Mathematics and Computer Science
Technical University of Denmark*

02619 Model Predictive Control - Lecture 4

Flow and Chemical Reaction in a Pipe



Chemical Reaction:



Flux for convective and diffusive flow:

$$N_A = vC_A + J_A \quad J_A = -D_A \frac{\partial C_A}{\partial z}$$

$$Accumulated = [C_A(t + \Delta t, z) - C_A(t, z)] S \Delta z$$

$$Influx = N_A(t, z) S \Delta t$$

$$Outflux = N_A(t, z + \Delta z) S \Delta t$$

$$Generated = R_A S \Delta z \Delta t$$

► Model (mass balance)

$$\frac{\partial C_A(t, z)}{\partial t} = -\frac{\partial N_A(t, z)}{\partial z} + R_A(t, z)$$

► Boundary conditions

$$z = 0 : \quad N_A(t, 0) = vC_{A,in}$$

$$z = L : \quad N_A(t, L) = vC_A(t, L)$$

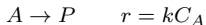
► Initial condition

$$t = 0 : \quad C_A(0, z) = C_{A0}(z)$$

► Flux

$$N_A(t, z) = \overbrace{vC_A(t, z)}^{\text{convection}} - \overbrace{D_A \frac{\partial C_A(t, z)}{\partial z}}^{\text{diffusion}}$$

► Stoichiometry and kinetics



► Production rates

$$R_A = -r$$

► Equidistant spatial discretization

$$z_j = \left(j - \frac{1}{2}\right) \Delta z \quad \Delta z = \frac{L}{N_z}$$

► Spatial discretization of partial differential equation (method of lines)

$$\frac{dC_{A,j}(t)}{dt} = -\frac{N_{A,j+1/2}(t) - N_{A,j-1/2}(t)}{\Delta z} + R_{A,j}(t) \quad j = 1, 2, \dots, N_z$$

► Fluxes

$$N_{A,j+1/2}(t) = vC_{A,in}(t) \quad j = 0$$

$$N_{A,j+1/2}(t) = vC_{A,j}(t) - D_A \frac{C_{A,j+1}(t) - C_{A,j}(t)}{\Delta z} \quad j = 1, 2, \dots, N_z - 1$$

$$N_{A,j+1/2}(t) = vC_{A,j}(t) \quad j = N_z$$

► Reaction rates

$$r_j(t) = kC_{A,j}(t) \quad j = 1, 2, \dots, N_z$$

► Production rates

$$R_{A,j}(t) = -r_j(t) \quad j = 1, 2, \dots, N_z$$

The model

- Equidistant spatial discretization

$$z_j = \left(j - \frac{1}{2}\right) \Delta z \quad \Delta z = \frac{L}{N_z}$$

- Spatial discretization of partial differential equation (method of lines)

$$\frac{dC_{A,j}(t)}{dt} = - \frac{N_{A,j+1/2}(t) - N_{A,j-1/2}(t)}{\Delta z} + R_{A,j}(t) \quad j = 1, 2, \dots, N_z$$

- Fluxes

$$\begin{aligned} N_{A,j+1/2}(t) &= v C_{A,in}(t) & j &= 0 \\ N_{A,j+1/2}(t) &= v C_{A,j}(t) - D_A \frac{C_{A,j+1}(t) - C_{A,j}(t)}{\Delta z} & j &= 1, 2, \dots, N_z - 1 \\ N_{A,j+1/2}(t) &= v C_{A,j}(t) & j &= N_z \end{aligned}$$

- Reaction rates

$$r_j(t) = k C_{A,j}(t) \quad j = 1, 2, \dots, N_z$$

- Production rates

$$R_{A,j}(t) = -r_j(t) \quad j = 1, 2, \dots, N_z$$

can be represented as

$$\begin{aligned} \dot{x}(t) &= f(x(t), u(t)) & x(t_0) &= x_0 \\ y(t) &= g(x(t)) \end{aligned}$$

with $x = [C_{A,1}; C_{A,2}; \dots, C_{A,N_z}]$, $u = C_{A,in}$, and $y = C_{A,out} = C_{A,N_z}$

$$\frac{dC_{A,1}}{dt} = \left(\frac{v}{\Delta z} \right) C_{A,in} + \left(-\frac{v + \frac{DA}{\Delta z}}{\Delta z} - k \right) C_{A,1} + \left(\frac{\frac{DA}{\Delta z}}{\Delta z} \right) C_{A,2}$$

$$\frac{dC_{A,j}}{dt} = \left(\frac{v + \frac{DA}{\Delta z}}{\Delta z} \right) C_{A,j-1} + \left(-\frac{v + 2\frac{DA}{\Delta z}}{\Delta z} - k \right) C_{A,j} + \left(\frac{\frac{DA}{\Delta z}}{\Delta z} \right) C_{A,j+1} \quad j = 2, \dots, N_z - 1$$

$$\frac{dC_{A,N_z}}{dt} = \left(\frac{v + \frac{DA}{\Delta z}}{\Delta z} \right) C_{A,N_z-1} + \left(-\frac{v + \frac{DA}{\Delta z}}{\Delta z} - k \right) C_{A,N_z}$$

$$\dot{x}(t) = A_c x(t) + B_c u(t)$$

$$y(t) = C_c x(t)$$

$$N_z = 5: x = [C_{A,1}; C_{A,2}; C_{A,3}; C_{A,4}; C_{A,5}], u = C_{A,in}, y = C_{A,out} = C_{A,5}$$

$$A_c = \begin{bmatrix} -\tilde{\alpha} & \gamma & 0 & 0 & 0 \\ \beta & -\alpha & \gamma & 0 & 0 \\ 0 & \beta & -\alpha & \gamma & 0 \\ 0 & 0 & \beta & -\alpha & \gamma \\ 0 & 0 & 0 & \beta & -\tilde{\alpha} \end{bmatrix} \quad B_c = \begin{bmatrix} \delta \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad C_c = [0 \quad 0 \quad 0 \quad 0 \quad 1]$$

$$\alpha = \beta + \gamma + k \quad \tilde{\alpha} = \beta + k \quad \beta = \frac{v + \frac{DA}{\Delta z}}{\Delta z} \quad \gamma = \frac{\frac{DA}{\Delta z}}{\Delta z} \quad \delta = \frac{v}{\Delta z}$$

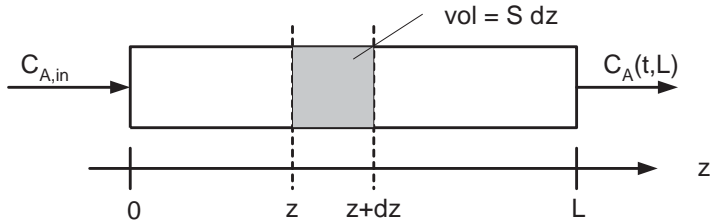
ZOH-discretization

$$x_{k+1} = A x_k + B u_k$$

$$y_k = C x_k$$

$$\begin{bmatrix} A & B \\ 0 & I \end{bmatrix} = \exp \left(\begin{bmatrix} A_c & B_c \\ 0 & 0 \end{bmatrix} T_s \right) \quad C = C_c$$

Flow and Chemical Reaction in a Pipe



Chemical Reaction:



Flux for convective and diffusive flow:

$$N_A = vC_A + J_A \quad J_A = -D_A \frac{\partial C_A}{\partial z}$$

$$\text{Accumulated} = [C_A(t + \Delta t, z) - C_A(t, z)] S \Delta z$$

$$\text{Influx} = N_A(t, z) S \Delta t$$

$$\text{Outflux} = N_A(t, z + \Delta z) S \Delta t$$

$$\text{Generated} = R_A S \Delta z \Delta t$$

► Model (mass balance)

$$\frac{\partial C_A(t, z)}{\partial t} = -\frac{\partial N_A(t, z)}{\partial z} + R_A(t, z)$$

► Boundary conditions

$$z = 0 : \quad N_A(t, 0) = vC_{A,in}$$

$$z = L : \quad N_A(t, L) = vC_A(t, L)$$

► Initial condition

$$t = 0 : \quad C_A(0, z) = C_{A0}(z)$$

► Flux

$$N_A(t, z) = \overbrace{vC_A(t, z)}^{\text{convection}} - \overbrace{D_A \frac{\partial C_A(t, z)}{\partial z}}^{\text{diffusion}}$$

► Stoichiometry and kinetics



► Production rates

$$R_A = -2r$$

► Equidistant spatial discretization

$$z_j = \left(j - \frac{1}{2}\right) \Delta z \quad \Delta z = \frac{L}{N_z}$$

► Spatial discretization of partial differential equation (method of lines)

$$\frac{dC_{A,j}(t)}{dt} = - \frac{N_{A,j+1/2}(t) - N_{A,j-1/2}(t)}{\Delta z} + R_{A,j}(t) \quad j = 1, 2, \dots, N_z$$

► Fluxes

$$N_{A,j+1/2}(t) = vC_{A,in}(t) \quad j = 0$$

$$N_{A,j+1/2}(t) = vC_{A,j}(t) - D_A \frac{C_{A,j+1}(t) - C_{A,j-1}(t)}{\Delta z} \quad j = 1, 2, \dots, N_z - 1$$

$$N_{A,j+1/2}(t) = vC_{A,j}(t) \quad j = N_z$$

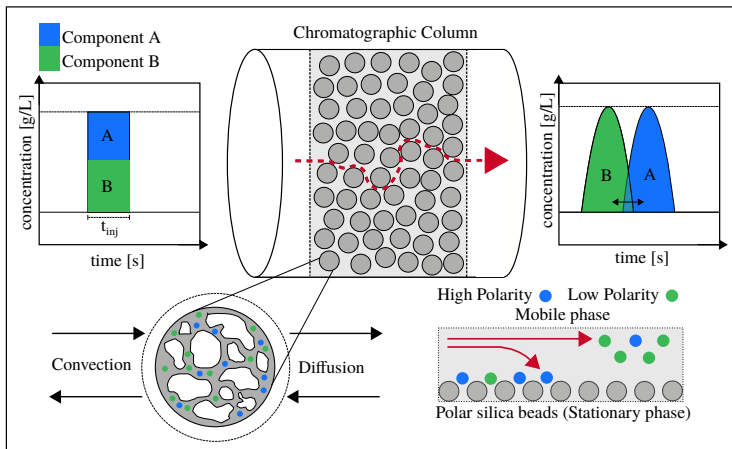
► Reaction rates

$$r_j(t) = k (C_{A,j}(t))^2 \quad j = 1, 2, \dots, N_z$$

► Production rates

$$R_{A,j}(t) = -2r_j(t) \quad j = 1, 2, \dots, N_z$$

Chromatography



Mathematical Model - Linear Equilibrium

- Mass balance

$$\frac{\partial}{\partial t} \bar{c}_i(t, z) = -\frac{\partial}{\partial z} \bar{N}_i(t, z)$$

- Flux

$$\bar{N}_i = \epsilon N_i$$

$$N_i = v c_i + J_i$$

- Diffusion

$$J_i = -D_i \frac{\partial}{\partial z} c_i$$

- Mobile and immobile phase

$$V \bar{c}_i = \epsilon V c_i + (1 - \epsilon) V q_i$$

is equivalent to

$$\bar{c}_i = \epsilon c_i + (1 - \epsilon) q_i$$

- Equilibrium (linear)

$$K_i = \frac{q_i}{c_i}$$

Mathematical Model - Linear Equilibrium

The equations

- Mass balance

$$\frac{\partial}{\partial t} \bar{c}_i(t, z) = - \frac{\partial}{\partial z} \bar{N}_i(t, z)$$

- Flux

$$\bar{N}_i = \epsilon N_i$$

$$N_i = v c_i + J_i$$

- Diffusion

$$J_i = -D_i \frac{\partial}{\partial z} c_i$$

- Mobile and immobile phase

$$V \bar{c}_i = \epsilon V c_i + (1 - \epsilon) V q_i$$

is equivalent to

$$\bar{c}_i = \epsilon c_i + (1 - \epsilon) q_i$$

- Equilibrium (linear)

$$K_i = \frac{q_i}{c_i}$$

correspond to

$$\left(1 + \frac{1 - \epsilon}{\epsilon} K_i\right) \frac{\partial}{\partial t} c_i = -v \frac{\partial}{\partial z} c_i + D_i \frac{\partial^2}{\partial z^2} c_i$$

$$q_i = K_i c_i$$

$$\bar{c}_i = \epsilon c_i + (1 - \epsilon) q_i$$

Mathematical Model - Linear Equilibrium

$$\left(1 + \frac{1-\epsilon}{\epsilon}K_i\right) \frac{\partial}{\partial t}c_i = -v\frac{\partial}{\partial z}c_i + D_i\frac{\partial^2}{\partial z^2}c_i$$

is a linear system of partial differential equations

$$\frac{\partial}{\partial t}c_i = a_i\frac{\partial}{\partial z}c_i + b_i\frac{\partial^2}{\partial z^2}c_i$$

with

$$a_i = \frac{-v}{1 + \frac{1-\epsilon}{\epsilon}K_i}$$

$$b_i = \frac{D_i}{1 + \frac{1-\epsilon}{\epsilon}K_i}$$

For short we write this as

$$\partial_t c_i = a_i \partial_z c_i + b_i \partial_{zz}^2 c_i$$

Mathematical Model - Linear Equilibrium

- Mathematical model:

$$t > 0, 0 < z < L : \quad \partial_t c_i = a_i \partial_z c_i + b_i \partial_{zz}^2 c_i$$

- Boundary conditions:

$$z = 0 : \quad N_i = v c_i - D_i \partial_z c_i = v c_{i,in}$$

$$z = L : \quad \partial_z c_i = 0$$

- Initial value condition:

$$t = 0 : \quad c_i(0, z) = c_{i,init}(z)$$

- Linear continuous-time and discrete-time state space model

$$\dot{x}(t) = A_c x(t) + B_c u(t) \quad x_{k+1} = A x_k + B u_k$$

$$y(t) = C x(t) \quad y_k = C x_k$$

► Mathematical model:

$$t > 0, 0 < z < L : \quad \left(1 + \frac{1-\epsilon}{\epsilon} K_i\right) \partial_t c_i = -\partial_z N_i, \quad N_i = v c_i - D_i \partial_z c_i$$

$$z = 0 : \quad N_i = v c_i - D_i \partial_z c_i = v c_{i,in}$$

$$z = L : \quad \partial_z c_i = 0$$

► Spatial discretization

$$\begin{aligned} \left(1 + \frac{1-\epsilon}{\epsilon} K_i\right) \frac{d}{dt} c_{i,1} &= -\frac{N_{i,3/2} - N_{i,1/2}}{\Delta z} \\ \left(1 + \frac{1-\epsilon}{\epsilon} K_i\right) \frac{d}{dt} c_{i,j} &= -\frac{N_{i,j+1/2} - N_{i,j-1/2}}{\Delta z}, \quad j = 2, \dots, N_z - 1 \\ \left(1 + \frac{1-\epsilon}{\epsilon} K_i\right) \frac{d}{dt} c_{i,N_z} &= -\frac{N_{i,N_z+1/2} - N_{i,N_z-1/2}}{\Delta z} \end{aligned}$$

► Flux

$$N_{i,1/2} = v c_{i,in}$$

$$N_{i,j+1/2} = v c_{i,j} - D_i \frac{c_{i,j+1} - c_{i,j}}{\Delta z}, \quad j = 1, 2, \dots, N_z - 1$$

$$N_{i,N_z+1/2} = v c_{i,N_z}$$

► Discretized system

$$\begin{aligned}\left(1 + \frac{1-\epsilon}{\epsilon} K_i\right) \frac{d}{dt} c_{i,1} &= \left(\frac{v}{\Delta z}\right) c_{i,in} + \left(-\frac{v + D_i/\Delta z}{\Delta z}\right) c_{i,1} + \left(\frac{D_i/\Delta z}{\Delta z}\right) c_{i,2} \\ \left(1 + \frac{1-\epsilon}{\epsilon} K_i\right) \frac{d}{dt} c_{i,j} &= \left(\frac{v + D_i/\Delta z}{\Delta z}\right) c_{i,j-1} + \left(-\frac{v + 2D_i/\Delta z}{\Delta z}\right) c_{i,j} + \left(\frac{D_i/\Delta z}{\Delta z}\right) c_{i,j+1} \\ \left(1 + \frac{1-\epsilon}{\epsilon} K_i\right) \frac{d}{dt} c_{i,N_z} &= \left(\frac{v + D_i/\Delta z}{\Delta z}\right) c_{i,N_z-1} + \left(-\frac{v + D_i/\Delta z}{\Delta z}\right) c_{i,N_z}\end{aligned}$$

► State space form

$$\dot{x}_i(t) = A_{c,i} x_i(t) + B_{c,i} u_i(t)$$

$$y_i(t) = C_{c,i} x_i(t)$$

$$N_z = 5$$

$$x_i = [c_{i,1}; c_{i,2}; c_{i,3}; c_{i,4}; c_{i,5}] \quad u_i = c_{i,in} \quad y_i = c_{i,N_z+1} = c_{i,N_z}$$

$$A_{c,i} = \begin{bmatrix} -\beta_i & \gamma_i & & & \\ \beta_i & -\alpha_i & & & \\ & \beta_i & \gamma_i & & \\ & & -\alpha_i & \gamma_i & \\ & & \beta_i & -\alpha_i & \gamma_i \\ & & & \beta_i & -\beta_i \end{bmatrix} \quad B_{c,i} = \begin{bmatrix} \delta_i \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad C_{c,i} = [0 \quad 0 \quad 0 \quad 0 \quad 1]$$

$$\alpha_i = \beta_i + \gamma_i \quad \beta_i = \frac{v + D_i/\Delta z}{\kappa_i} \quad \delta_i = \frac{v}{\kappa_i} \quad \gamma_i = \frac{D_i/\Delta z}{\kappa_i} \quad \kappa_i = 1 + \frac{1-\epsilon}{\epsilon} K_i$$

- State-space model
 - Continuous time

$$\begin{aligned}\dot{x}_i(t) &= A_{c,i}x_i(t) + B_{c,i}u_i(t), \quad x_{i,k} = x_i(t_k) \quad u_i(t) = u_{i,k} \text{ for } t_k \leq t < t_{k+1} \\ y_i(t) &= C_c x_i(t)\end{aligned}$$

- Discrete time

$$\begin{aligned}x_{i,k+1} &= A_i x_{i,k} + B_i u_{i,k} \\ y_{i,k} &= C_i x_{i,k} \qquad C_i = C_{c,i}\end{aligned}$$

- Explicit-Euler discretization

$$A_i = I + \Delta t A_{c,i} \quad B_i = \Delta t B_{c,i}$$

- Implicit-Euler discretization

$$A_i = (I - \Delta t A_{c,i})^{-1} \quad B_i = \Delta t (I - \Delta t A_{c,i})^{-1} B_{c,i}$$

- Trapezoidal discretization

$$A_i = \left(I - \frac{1}{2} \Delta t A_{c,i} \right)^{-1} \left(I + \frac{1}{2} \Delta t A_{c,i} \right) \quad B_i = \Delta t \left(I - \frac{1}{2} \Delta t A_{c,i} \right)^{-1} B_{c,i}$$

- Exact discretization

$$A_i = \exp(A_{c,i} \Delta t) \quad B_i = \int_0^{\Delta t} \exp(A_{c,i} s) B_{c,i} ds$$

$$\begin{bmatrix} A_i & B_i \\ 0 & I \end{bmatrix} = \exp \left(\begin{bmatrix} A_{c,i} & B_{c,i} \\ 0 & 0 \end{bmatrix} \Delta t \right)$$

Stochastic Discrete-Time Model and Kalman Filter

$$\begin{aligned}x_{i,k+1} &= A_i x_{i,k} + B_i(u_{i,k} + w_{i,k}) & w_{i,k} &\sim N_{iid}(0, Q_i) \\y_{i,k} &= C_i x_{i,k} + v_{i,k} & v_{i,k} &\sim N_{iid}(0, R_i)\end{aligned}$$

Dynamic Kalman filter

$$\begin{aligned}\hat{y}_{i,k|k-1} &= C_i \hat{x}_{i,k|k-1} \\e_{i,k} &= y_{i,k} - \hat{y}_{i,k|k-1} \\R_{e,i,k} &= C_i P_{i,k|k-1} C_i' + R_i \\K_{i,k} &= P_{i,k|k-1} C_i' R_{e,i,k}^{-1} \\\hat{x}_{i,k|k} &= \hat{x}_{i,k|k-1} + K_{i,k} e_{i,k} \\P_{i,k|k} &= P_{i,k|k-1} - K_{i,k} R_{e,i,k} K_{i,k}' = (I - K_{i,k} C_i) P_{i,k|k-1} (I - K_{i,k} C_i)' + K_{i,k} R_i K_{i,k}'\end{aligned}$$

One-step predictor

$$\begin{aligned}\hat{x}_{i,k+1|k} &= A_i \hat{x}_{i,k|k} + B_i \hat{u}_{i,k|k} \\P_{i,k+1|k} &= A_i P_{i,k|k} A_i' + B_i Q_i B_i'\end{aligned}$$

j-step predictor

$$\begin{aligned}\hat{x}_{i,k+1+j|k} &= A_i \hat{x}_{i,k+j|k} + B_i \hat{u}_{i,k+j|k} \\P_{i,k+1+j|k} &= A_i P_{i,k+j|k} A_i' + B_i Q_i B_i'\end{aligned}$$

- The linear ordinary differential equation system (deterministic)

$$dx_i(t) = (A_{c,i}x_i(t) + B_{c,i}u_i(t)) dt$$

can be expressed as

$$dx_i(t) = (A_{c,i}x_i(t) + B_{c,i}u_i(t)) dt$$

- Linear stochastic differential equation system (stochastic)

$$\begin{aligned} dx_i(t) &= (A_{c,i}x_i(t) + B_{c,i}u_i(t)) dt + B_{c,i}\sigma_i d\omega_i(t) \\ &= A_{c,i}x_i(t)dt + B_{c,i}(u_i(t)dt + \sigma_i d\omega_i(t)) \end{aligned}$$

$d\omega_i(t) \sim N_{iid}(0, dt)$ such that $\omega_i(t)$ is a standard Wiener process.

- Exact discretization for $u_i(t) = u_{i,k}$ when $t_k \leq t < t_{k+1}$:

$$x_{i,k+1} = A_i x_{i,k} + B_i u_{i,k} + w_{i,k} \quad w_{i,k} \sim N_{iid}(0, Q_i)$$

$$A_i = \exp(A_{c,i}\Delta t) \quad B_i = \int_0^{\Delta t} \exp(A_{c,i}s) B_{c,i} ds$$

$$Q_i = \int_0^{\Delta t} \exp(A_{c,i}s) B_{c,i} \sigma_i \sigma_i' B_{c,i}' \exp(A_{c,i}'s) ds$$

$$\begin{bmatrix} A_i & B_i \\ 0 & I \end{bmatrix} = \exp \left(\begin{bmatrix} A_{c,i} & B_{c,i} \\ 0 & 0 \end{bmatrix} \Delta t \right)$$

$$\begin{bmatrix} \Phi_{i,11} & \Phi_{i,12} \\ 0 & \Phi_{i,22} \end{bmatrix} = \exp \left(\begin{bmatrix} -A_{c,i} & B_{c,i} \sigma_i \sigma_i' B_{c,i}' \\ 0 & A_{c,i}' \end{bmatrix} \Delta t \right)$$

$$Q_i = \Phi_{i,22}' \Phi_{i,12}$$

- Discrete measurement equation

$$y_{i,k} = C_i x_{i,k} + v_{i,k} \quad v_{i,k} \sim N_{iid}(0, R_i)$$

- We can apply the discrete-time Kalman filter for the discrete-time system corresponding to the continuous-discrete system

Kalman filter for continuous-discrete systems

► Continuous-discrete system

$$dx_i(t) = A_{c,i}x_i(t)dt + B_{c,i}(u_i(t)dt + \sigma_i d\omega_i(t)) \quad d\omega_i(t) \sim N_{iid}(0, Idt)$$

$$y_i(t_k) = C_i x_i(t_k) + v_i(t_k) \quad v_i(t_k) \sim N_{iid}(0, R_i)$$

► Equivalent discrete-discrete system

$$x_{i,k+1} = A_i x_{i,k} + B_i u_{i,k} + w_{i,k} \quad w_{i,k} \sim N_{iid}(0, Q_i)$$

$$y_{i,k} = C_i x_{i,k} + v_{i,k} \quad v_{i,k} \sim N_{iid}(0, R_i)$$

► Dynamic Kalman filter for the discrete-discrete system Filter

$$\hat{y}_{i,k|k-1} = C_i \hat{x}_{i,k|k-1}$$

$$e_{i,k} = y_{i,k} - \hat{y}_{i,k|k-1}$$

$$R_{e,i,k} = C_i P_{i,k|k-1} C_i' + R_i$$

$$K_{i,k} = P_{i,k|k-1} C_i' R_{e,i,k}^{-1}$$

$$\hat{x}_{i,k|k} = \hat{x}_{i,k|k-1} + K_{i,k} e_{i,k}$$

$$P_{i,k|k} = P_{i,k|k-1} - K_{i,k} R_{e,i,k} K_{i,k}' = (I - K_{i,k} C_i) P_{i,k|k-1} (I - K_{i,k} C_i)' + K_{i,k} R_i K_{i,k}'$$

One-step predictor

$$\hat{x}_{i,k+1|k} = A_i \hat{x}_{i,k|k} + B_i \hat{u}_{i,k|k}$$

$$P_{i,k+1|k} = A_i P_{i,k|k} A_i' + Q_i$$

j-step predictor

$$\hat{x}_{i,k+1+j|k} = A_i \hat{x}_{i,k+j|k} + B_i \hat{u}_{i,k+j|k}$$

$$P_{i,k+1+j|k} = A_i P_{i,k+j|k} A_i' + Q_i$$