Novosibirsk State Technical University

NETI

II International Scientific Conference

Advanced Technologies in Aerospace, Mechanical and Automation Engineering - MIST: Aerospace - 2019

Modeling and Simulation of Chemical Processes Using the Hybrid Methodology

Yury V. Shornikov
Evgeny A. Popov

Krasnoyarsk, Russia, 2019

Hybrid Dynamical Systems

Explicit DAEs with constraints

$$y' = f(x, y, t),$$

$$x = \varphi(x, y, t),$$

$$pr : g(x, y, t) < 0,$$

$$t \in [t_0, t_k], x(t_0) = x_0, y(t_0) = y_0,$$

where $x \in R^{N_x}, y \in R^{N_y}, t \in R,$

$$f : R^{N_x} \times R^{N_y} \times R \to R^{N_y},$$

$$\varphi : R^{N_x} \times R^{N_y} \times R \to R^{Nx},$$

$$g : R^{N_x} \times R^{N_y} \times R \to R^{S}.$$

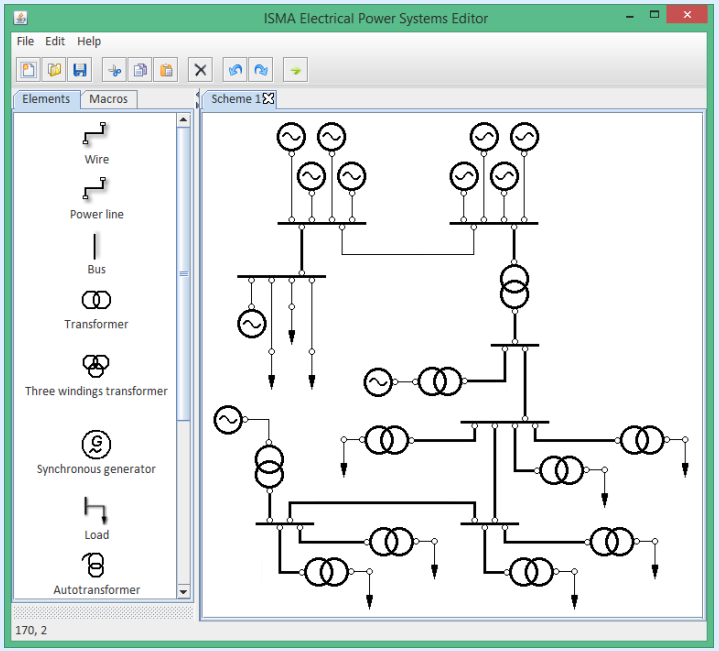
ISMA Modeling and Simulation Environment

Modeling languages:

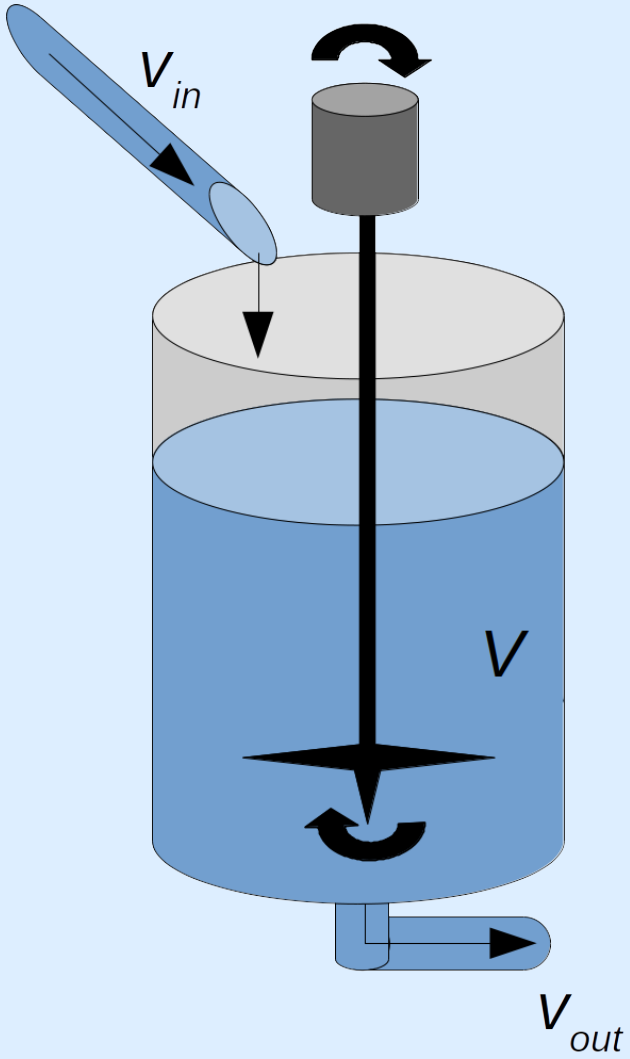
- Textual general-purpose language LISMA;
- Block-textual diagrams;
- Harel statecharts;
- Domain-specific languages.

```
h1′ = (1 / S) * (Qp – Q1 – Q2 – V3 * Q3);
h2′ = (1 / S) * (Q2 + V3 * Q3 – V4 * Q4);

state st1 (h1 <= hv3) {
    V3 = 0;
} from init, st2;

state st2 (h1 > hv3) {
    V3 = 1;
} from init, st1;
```

```
C2H6=k1=>CH3+CH3;
CH3+C2H6=k2=>CH4+C2H5;
```



Continuous Ideally Stirred-Tank Reactor



$$\frac{dC_A}{dt} = \frac{v_{in}}{V} C_{A_{in}} - \frac{v_{out}}{V} C_A - k_1 C_A,$$

$$\frac{dC_B}{dt} = \frac{v_{in}}{V} C_{B_{in}} - \frac{v_{out}}{V} C_B + k_1 C_A - k_2 C_B,$$

$$\frac{dC_C}{dt} = -\frac{v_{out}}{V} C_C + k_2 C_B,$$

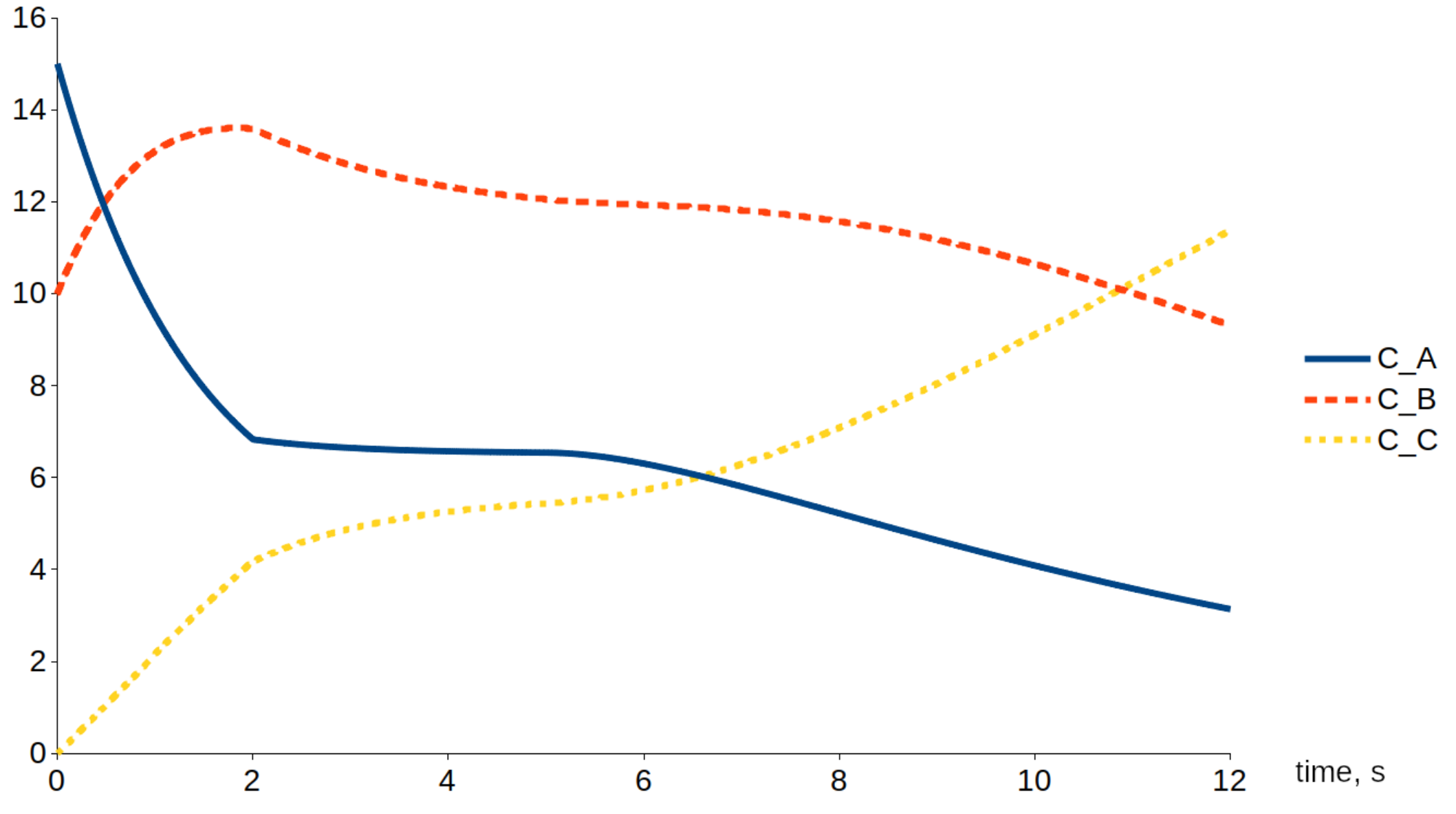
$$k_1 = 5.073 \cdot 10^8 \cdot e^{-\frac{10^5}{RT}},$$

$$k_2 = 1.34 \cdot 10^8 \cdot e^{-\frac{9.8 \cdot 10^4}{RT}}.$$

Computer Model in LISMA_PDE

```
const C_A_IN = 15.0, C_B_IN = 10.0; // inflow concentrations
const V = 1.0; // reactor volume
const R = 8.314; // universal gas constant

vIn = 0.2;          // inflow speed
vOut = 0.21;    // outflow speed

// reactor dynamics
cA' = vIn / V * C_A_IN - vOut / V * cA - k1 * cA;
cA(t0) = 15.0;
cB' = vIn / V * C_B_IN - vOut / V * cB + k1 * cA - k2 * cB;
cB(t0) = 10.0;
cC' = -vOut / V * cC + k2 * cB;
cC(t0) = 0.0;

k1 = 5.073E8 * exp(-1E5 / (R * temp));
k2 = 1.34E8 * exp(-9.8E4 / (R * temp));

// temperature
temp' = 0;
temp(t0) = 580.0;

const EVENT1_TIME = 2.0, EVENT2_TIME = 5.0;

// first event
state mode1(TIME >= EVENT1_TIME and TIME < EVENT2_TIME)
{
    vIn = 0.4;
    vOut = 0.42;
}
from init;

// second event
state mode2(TIME >= EVENT2_TIME)
{
    temp' = 5.0;
}
from mode1;
```

Simulation Results



Novosibirsk State Technical University

NETI

II International Scientific Conference

Advanced Technologies in Aerospace, Mechanical and Automation Engineering - MIST: Aerospace - 2019

Modeling and Simulation of Chemical Processes Using the Hybrid Methodology

Yury V. Shornikov
Evgeny A. Popov

Krasnoyarsk, Russia, 2019