Design and Control of Microchemical Plants

Shinji Hasebe

Department of Chemical Engineering,
Kyoto University, Japan

The International Symposium

on

Process Systems

Engineering

PSE'82

Kyoto International Conference Hall

Kyoto Japan

August 23—27,1982

Keynote

T. Takamatsu
R. W. H. Sargent
R. S. H. Mah
A. W. Westerberg
T. Umeda
E. O'Shima
G. Stephanopoulos
W. H. Ray
D. G. Fisher
M. Morari
I. E. Grossmann
D. W. T. Rippin
R. L. Motard
L. T. Fan
C. McGreavy

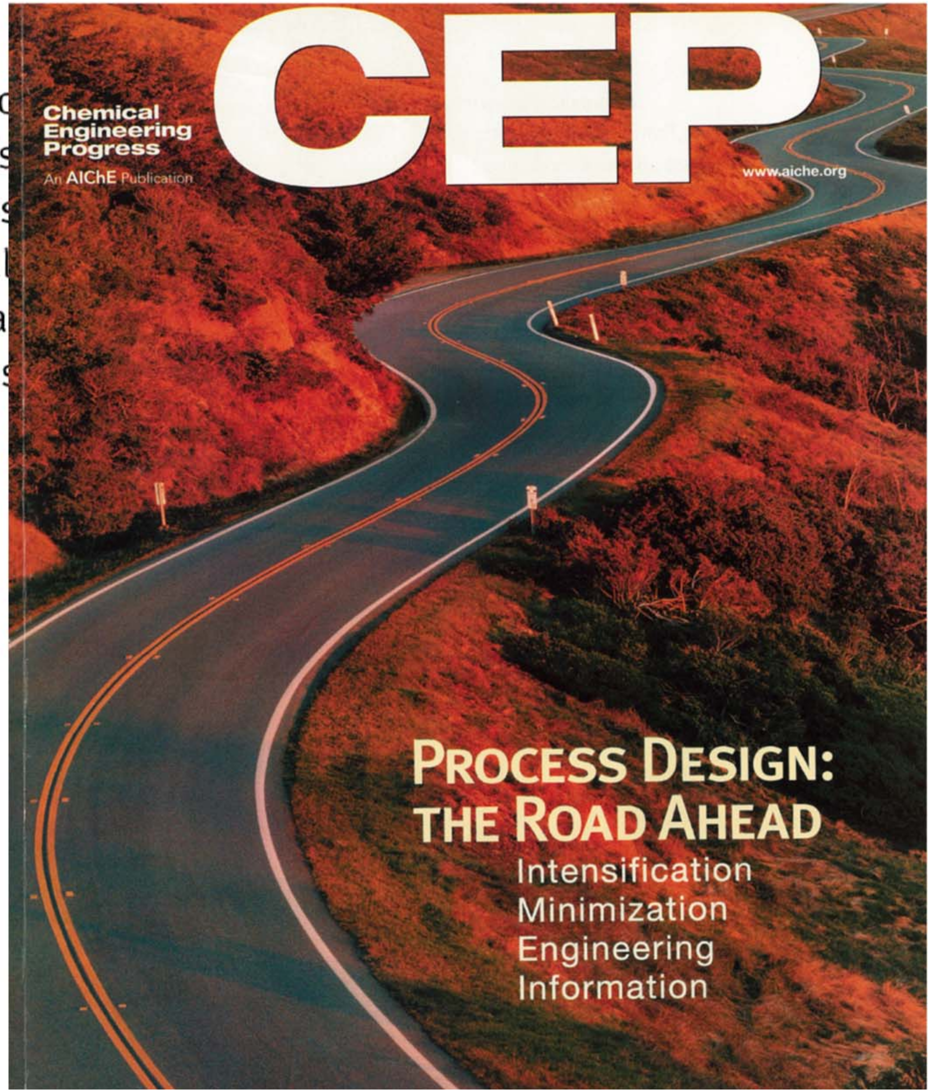
Contents

1. Why Micro Systems?
2. Feature of Design Problem of MCP
3. Contribution of PSE

Process Intensification: Transforming Chemical Engineering

Andrzej I. Stankiewicz,
DSM Research/Delft University of Technology
Jacob A. Moulijn,
Delft University of Technology

Emerging equipment, pro
and operational methods
improvements in process
their size and dramatical
These developments ma
of some traditional types
whole unit operations.



CEP, Jan. 2000

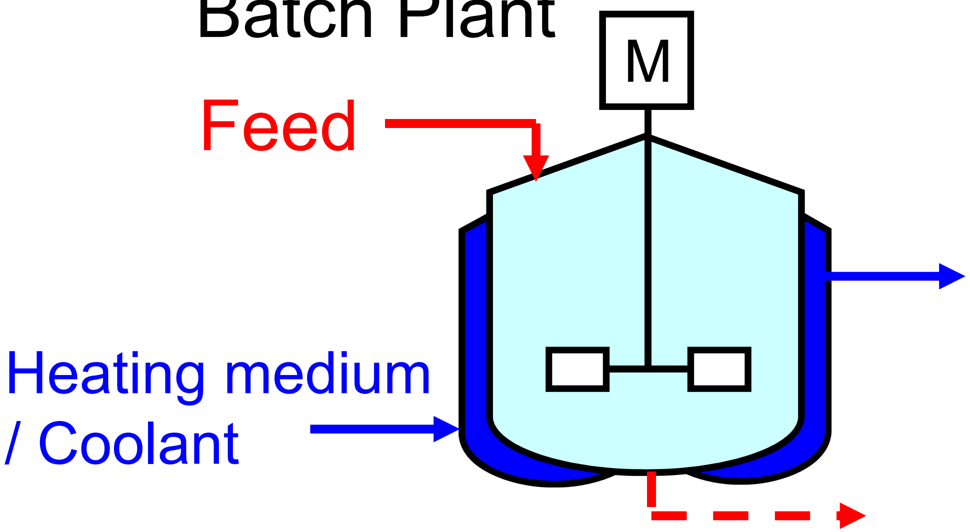
New Direction in Chemical Industries

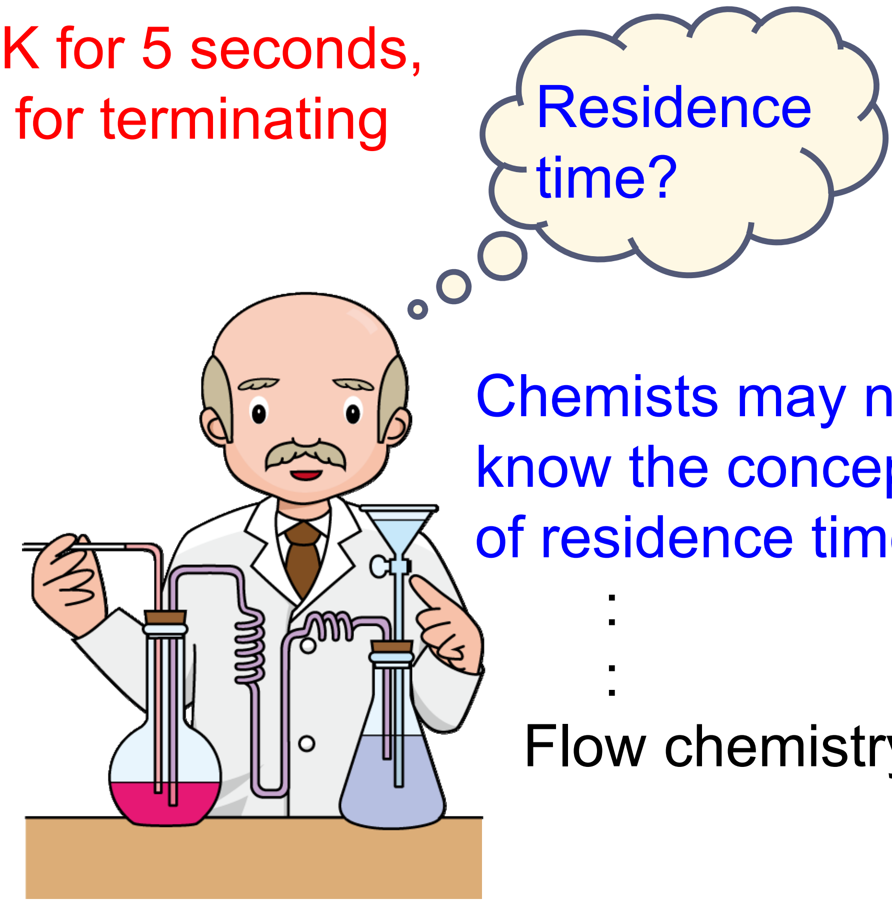
Production of low volume and high value added products

- Precise control on temperature, flow pattern and residence time, etc.

Mix A and B within 1 second, and heat up to 400 K within 2 seconds, keep the temperature at 400 K for 5 seconds, then cool down to 300 K within 1 second for terminating the reaction.

Batch Plant





Chemists may not know the concept of residence time.

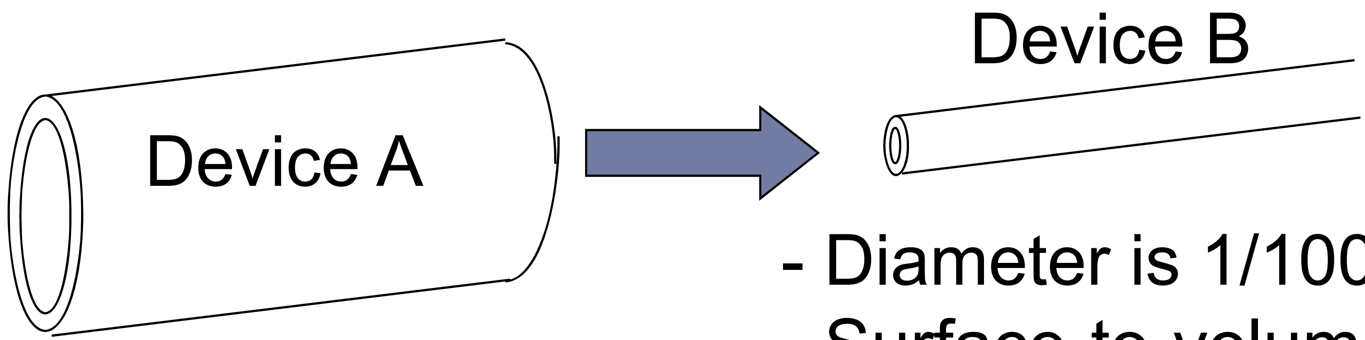
:

:

Flow chemistry

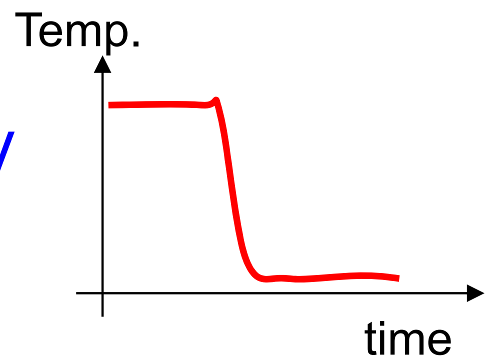
Characteristics of Micro Devices (1)

(1) Large surface-to-volume ratio



- Diameter is 1/100 of device A.
- Surface-to-volume ratio is 100 times larger than device A.

Efficient heat transfer through the wall
→ temperature can be controlled precisely



Temperature Control

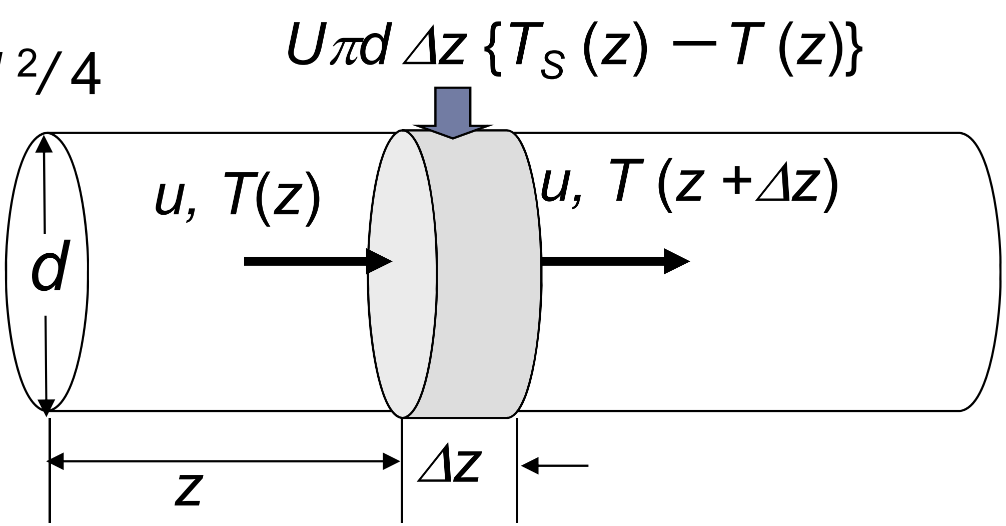
Enthalpy balance of heat exchanger

Increase rate of enthalpy = Heat entered with input flow − Heat removed with output flow + Heat entered from wall

$$0 = Su\rho c_p T(z) - Su\rho c_p T(z+\Delta z) + U\pi d\Delta z\{T_S(z) - T(z)\}$$

$$\frac{dT}{dz} = \frac{4U}{du\rho c_p}(T_S - T)$$

$S = \pi d^2/4$



S :cross-sectional area
u :mean velocity
ρ :liquid density
c_p :specific heat capacity
U : overall heat transfer coefficient
T_s :environmental temperature

Temperature Profile in Heat Exchanger

[Problem 1]

1) Solve Eq. (1) under the condition where r, v, ρ, c_p, U, T_s are constant.

$$\frac{dT(z)}{dz} = \frac{2U}{rv\rho c_p}\{T_s - T(z)\} \qquad (1)$$

2) Plot the temperature profile in the heat exchanger for following two cases:

<Case 1>

Inner diameter = 25 mm

<Case 2>

Inner diameter = 0.25 mm

The other conditions are given in the right box.

Length: L = 1 m

Feed liquid

Temperature: $T(0)$ = 100 °C

Feed velocity: v = 0.1 m/s

Density: ρ = 1000 kg/m^3

Specific heat capacity: c_p = 4.0 kJ/(kg K)

Wall temperature: T_s = 25 °C

Overall heat transfer coefficient:

U = 1.0 kJ/(m^2 s K)

Temperature Profile (Answer 1)

$$T(z) = T_S + (T(0) - T_S)\exp\left(-\frac{2U}{rv\rho c_p}z\right)$$

Case 1 ($2r$ = 25 mm)

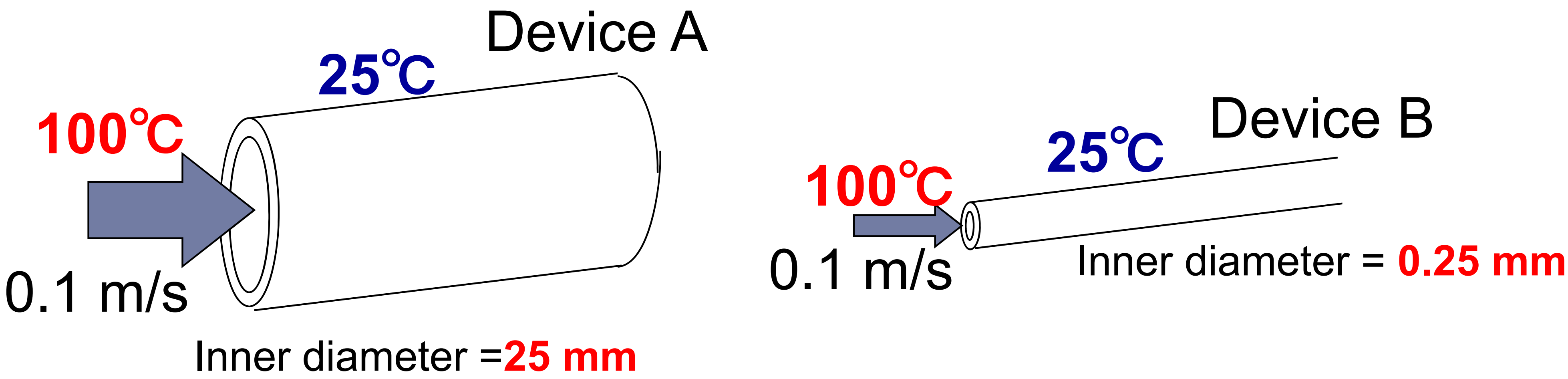
$$T(z) = 25 + 75\mathrm{e}^{-0.4z}$$

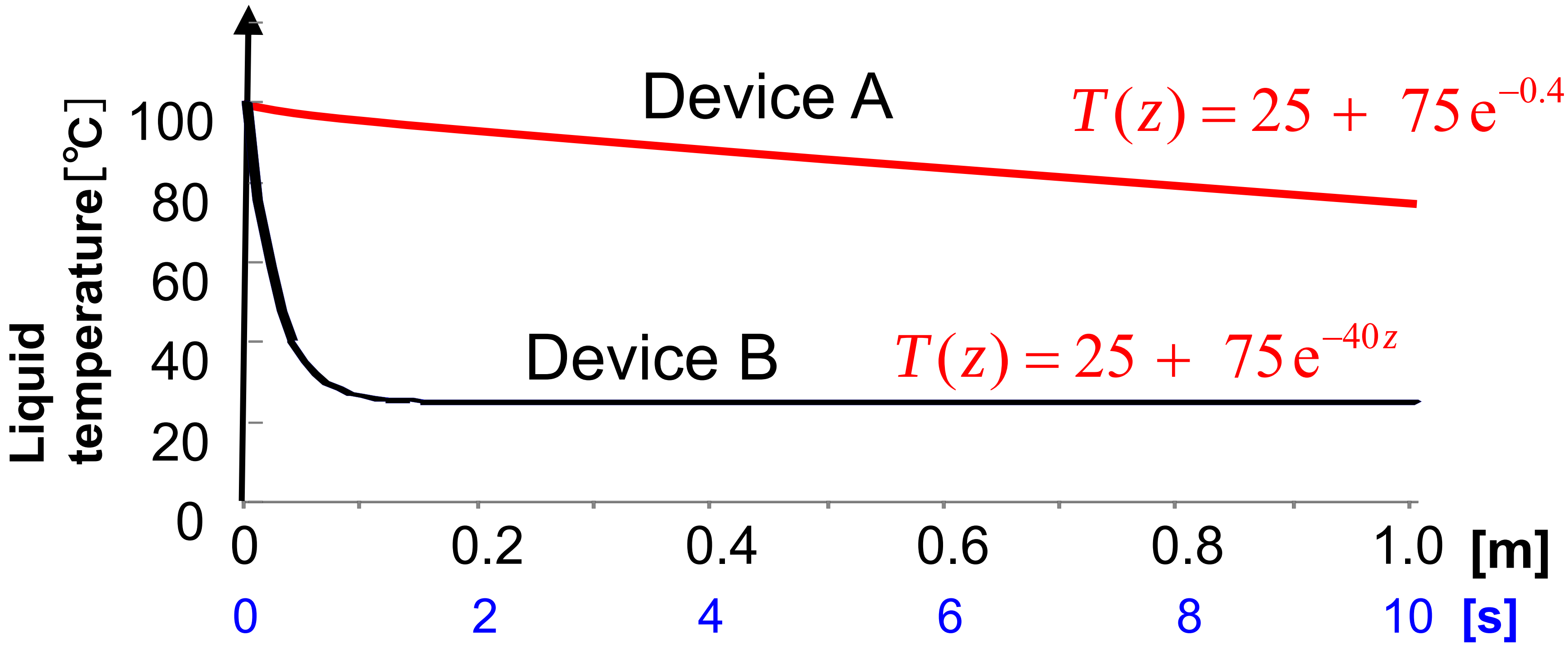
Case 2 ($2r$ = 0.25 mm)

$$T(z) = 25 + 75\mathrm{e}^{-40z}$$

Reactor length: L = 1 m
Feed liquid
Temperature: T (0) = 100 °C
Feed velocity: v = 0.1 m/s
Density: ρ = 1000 kg/m^3
Specific heat capacity: c_p = 4.0 kJ/(kg K)
Wall temperature: T_s = 25 °C
Overall heat transfer coefficient:
U = 1.0 kJ/(m^2 s K)

Temperature Profile (Answer 2)





Large Surface-to-Volume Ratio

Highly exothermic reaction (ex. combustion)

To avoid hot spot,

- Operate at low temperature (e.g. - 30 ℃, - 80 ℃)
- Dilute reactant with solvent
- Feed reactant slowly (Batch reactor)

Artificially slow down the reaction rate

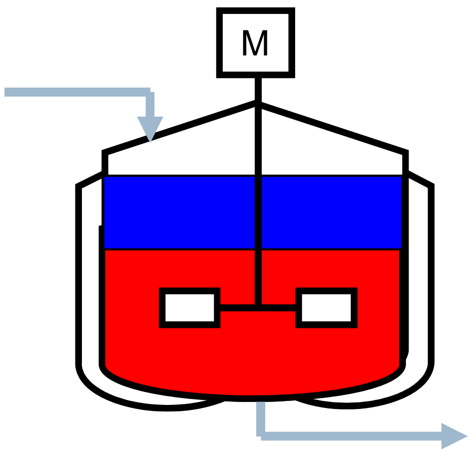
By using micro reactor, ・・・

Characteristics of Micro Devices

1) Large surface-to-volume ratio

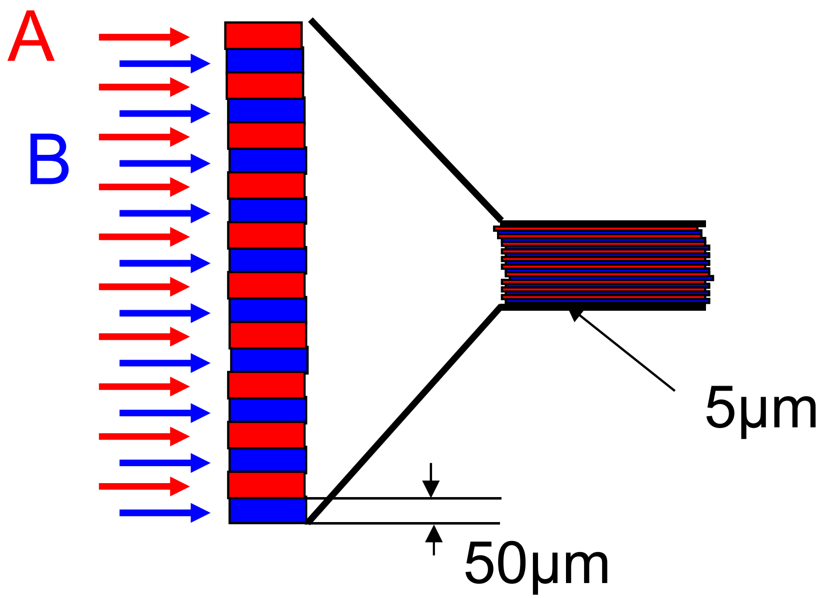
2) Rapid mixing

Conventional vessel



It is not easy to mix the oil and water in the order of a few micro meters.

Micro mixer



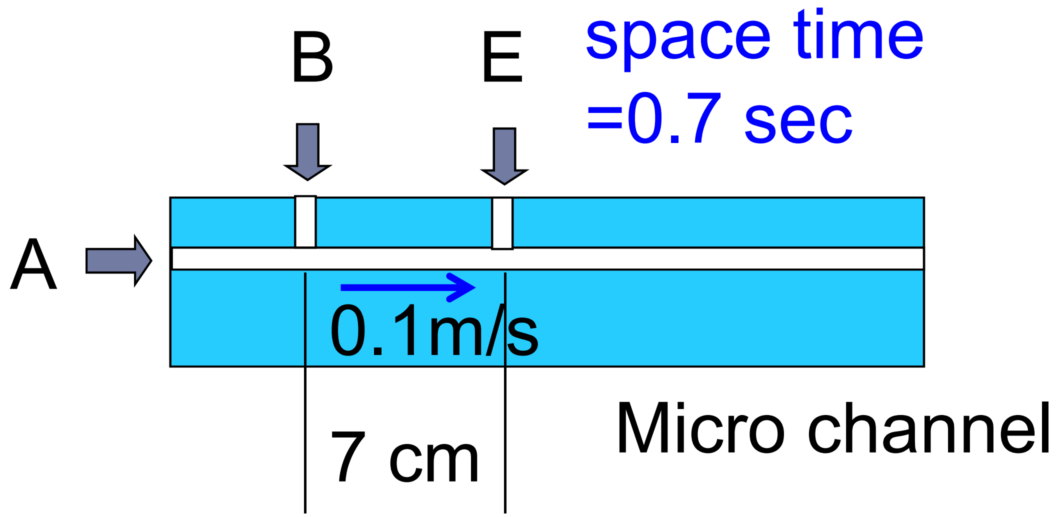
Mixing is finished instantaneously

Rapid Mixing improves the selectivity

Characteristics of Micro Devices

1) Large surface-to-volume ratio
2) Rapid Mixing
3) **Residence time control**

$A + B \rightarrow C$
$C + E \rightarrow F$: Product
$2C \rightarrow D$: Byproduct



Space time of 0.001 sec. is now available.

We can handle unstable intermediate.

Characteristics of Micro Devices

1) Large surface-to-volume ratio
2) Rapid mixing
3) Residence time control

↓

In order to use these characteristics effectively, new design and operation procedures are required.

Contents

1. Why Micro Systems?
2. Feature of Design Problem of MCP
3. Contribution of PSE

Micro Chemical Plants
Bridge between the Micro and Macro

Chemical Engineering Science (Micro)

Analysis of phenomena on nano-scale

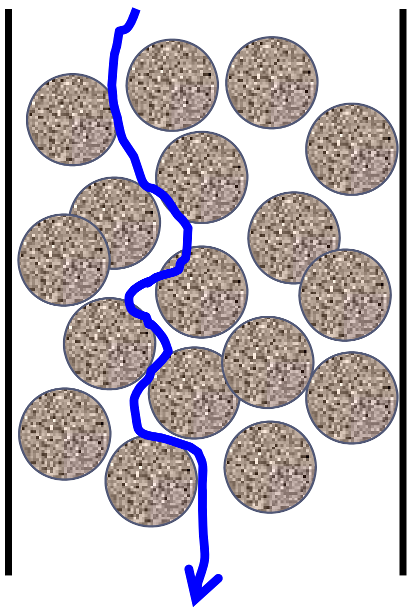
New results

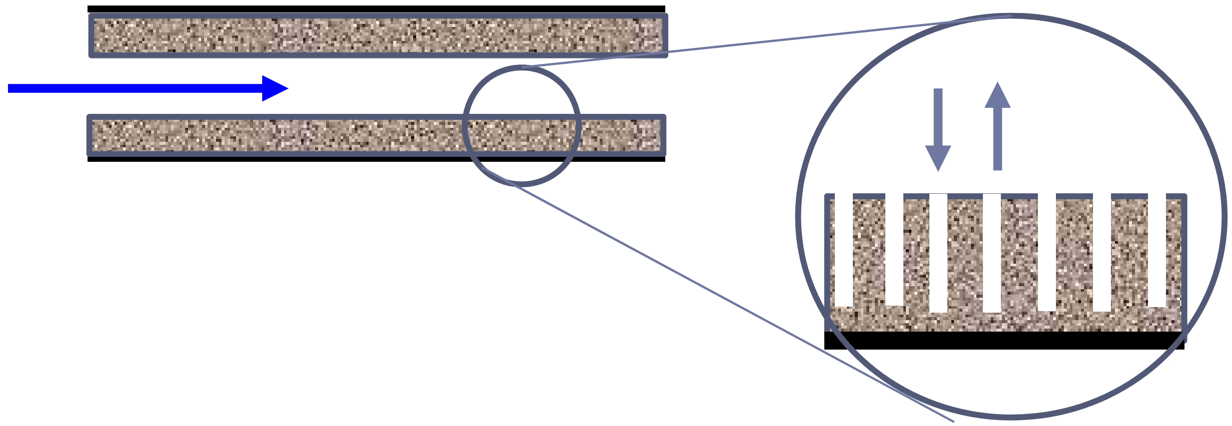
Gap

Process Systems Engineering (Macro)

Process design using simple model

- Lumped parameter system
- Overall heat transfer coefficient
- Perfect mixing or piston flow





Micro Chemical Plants

Bridge between the Micro and Macro

Chemical Engineering Science (Micro)

Analysis of phenomena on nano-scale

New results

Gap

Process Systems Engineering (Macro)

Process design using simple model

- Lumped parameter system
- Overall heat transfer coefficient
- Perfect mixing or piston flow

Design of micro chemical plants

- Detailed model
- Embed the results of CES

Innovation of process design

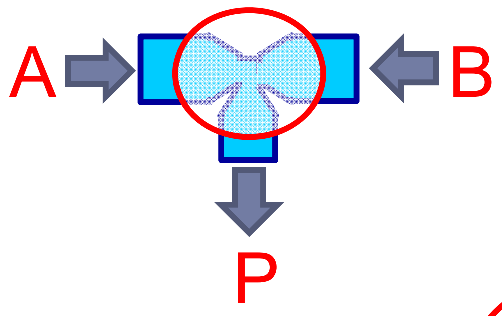
Design of Micro Device

Conventional design problem

Each unit operation is modeled as a lumped parameter system, i.e. the values do not depend on the location in the device.

⇨ Design variables are size and volume of the device

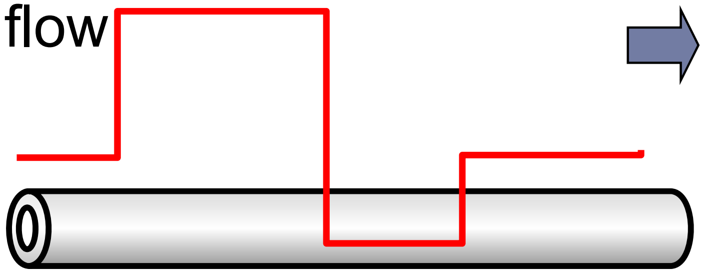
Design of micro devices

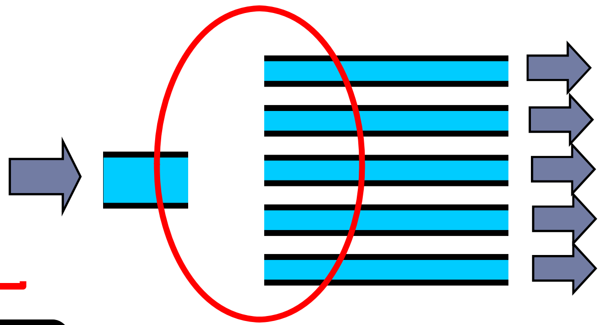


- Mixing of two kinds of materials

- Distribution of a stream

- Temperature control of a flow

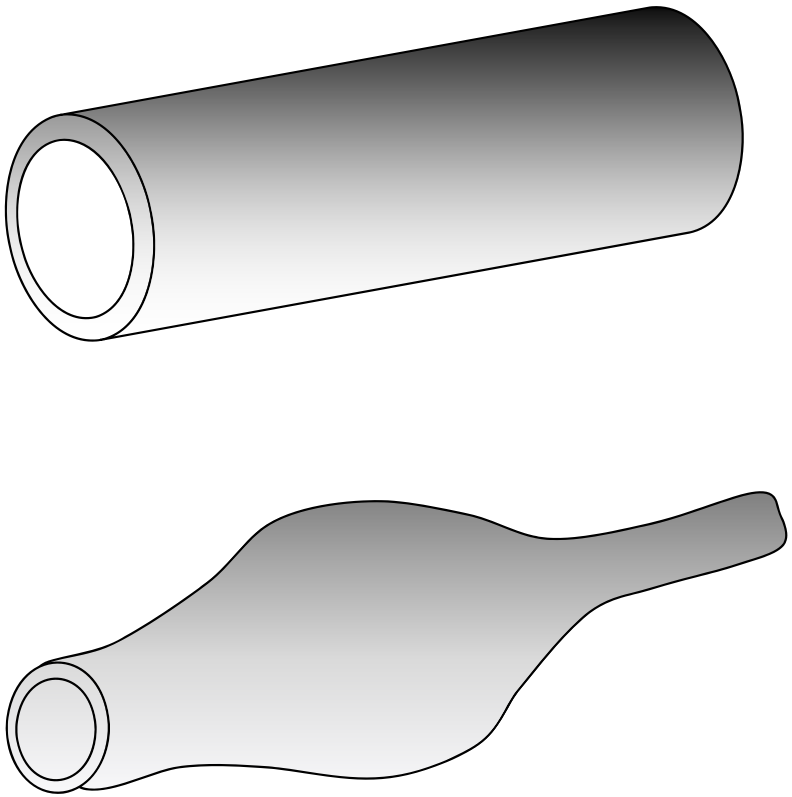




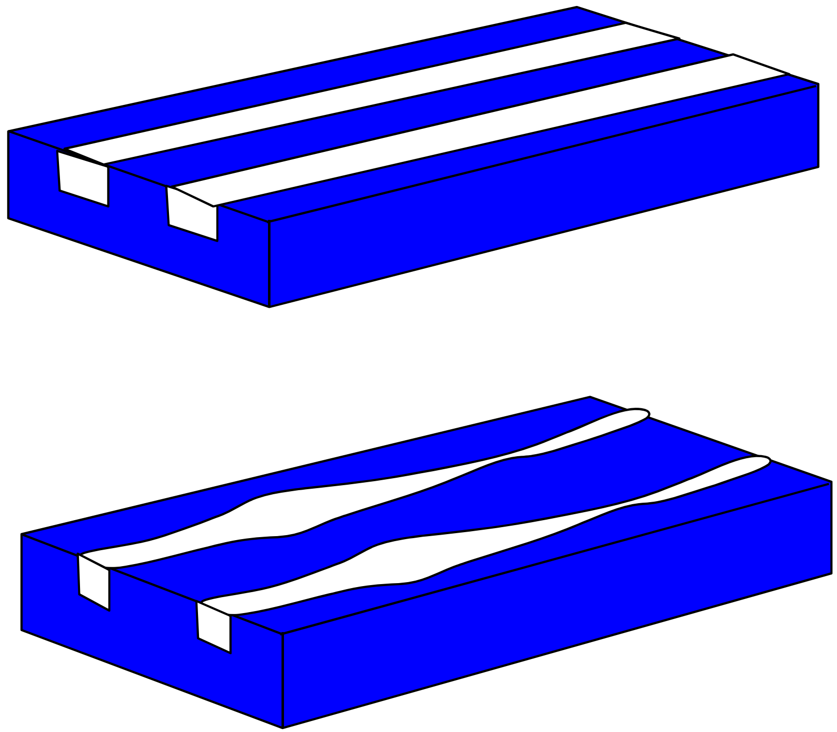
The shape of the device is an important design variable.

Shape of the Channel

Tube in
Conventional Reactor



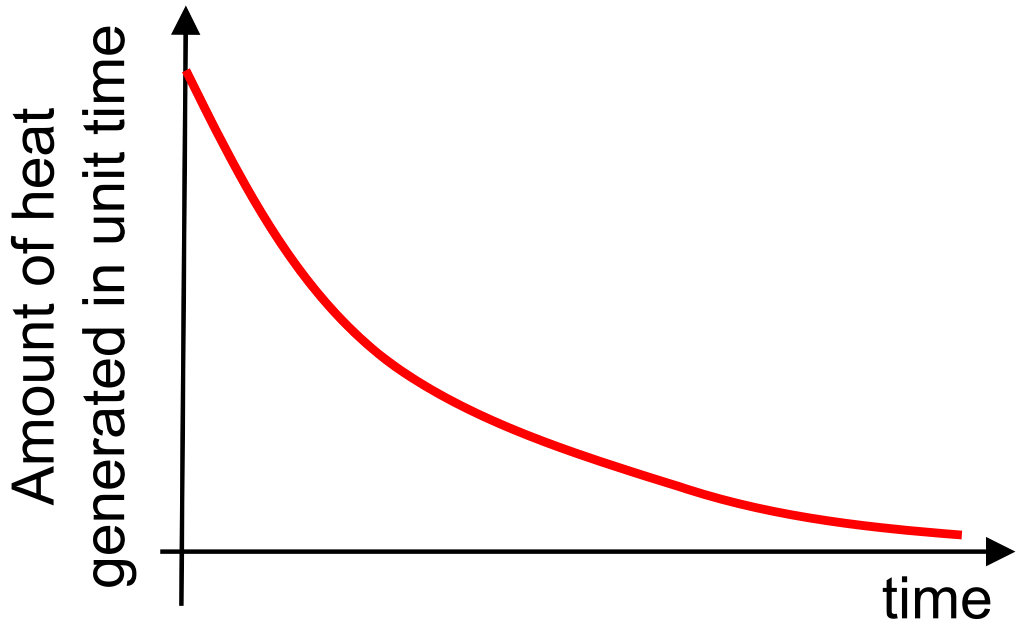
Channel in
Micro Reactor



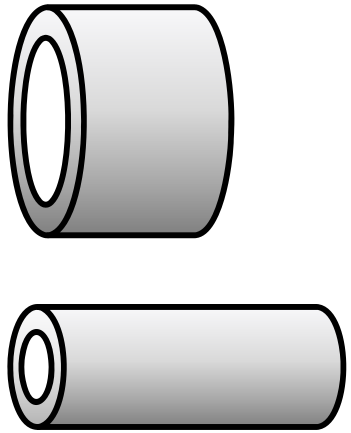
+ 3D Printer

Ex.) Highly Exothermic Reaction

Design a microdevice so that the temperature in the reactor is constant.



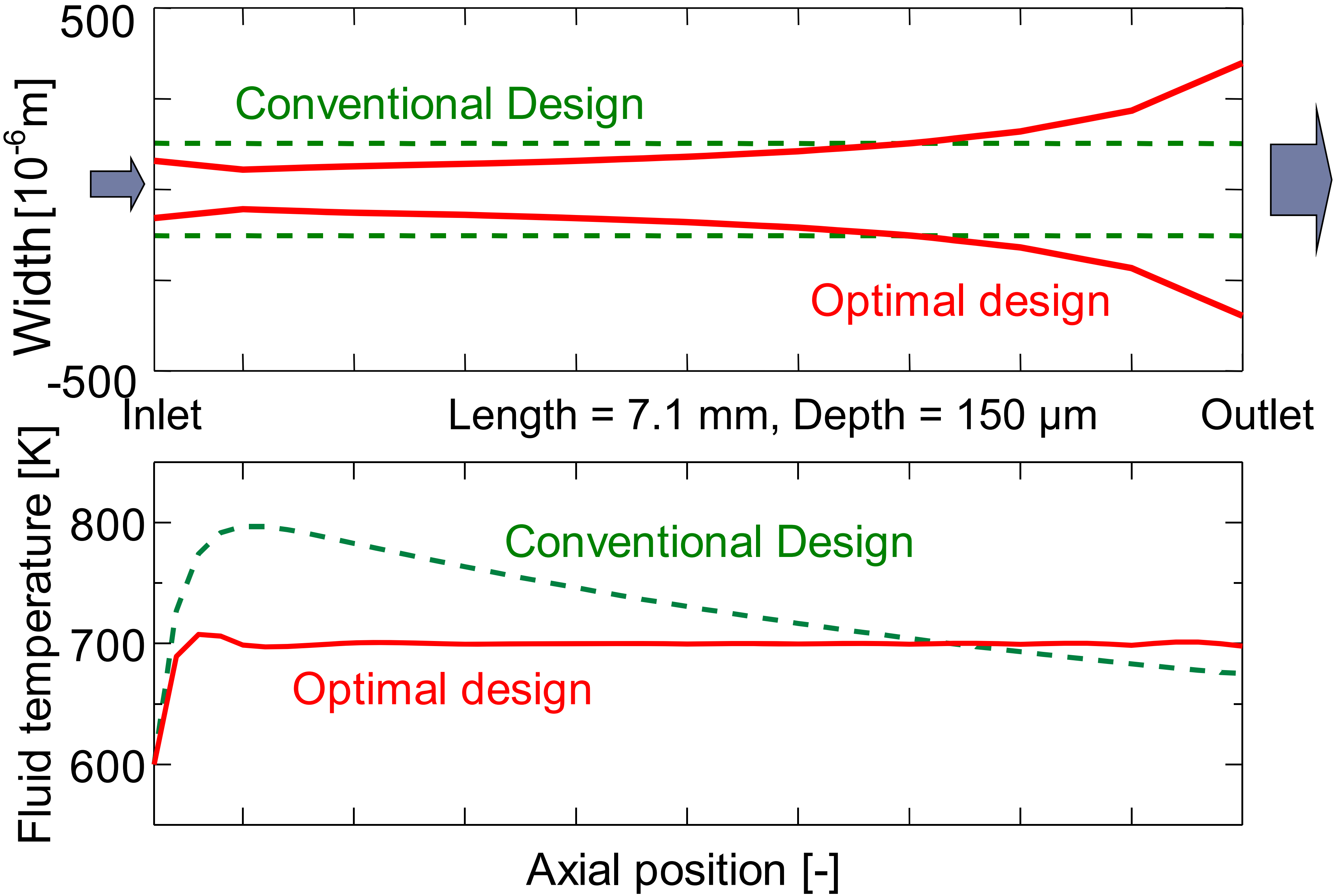
$Q = UA\Delta T$



Surface area per unit volume can be changed.

Channel Design of Microreactor

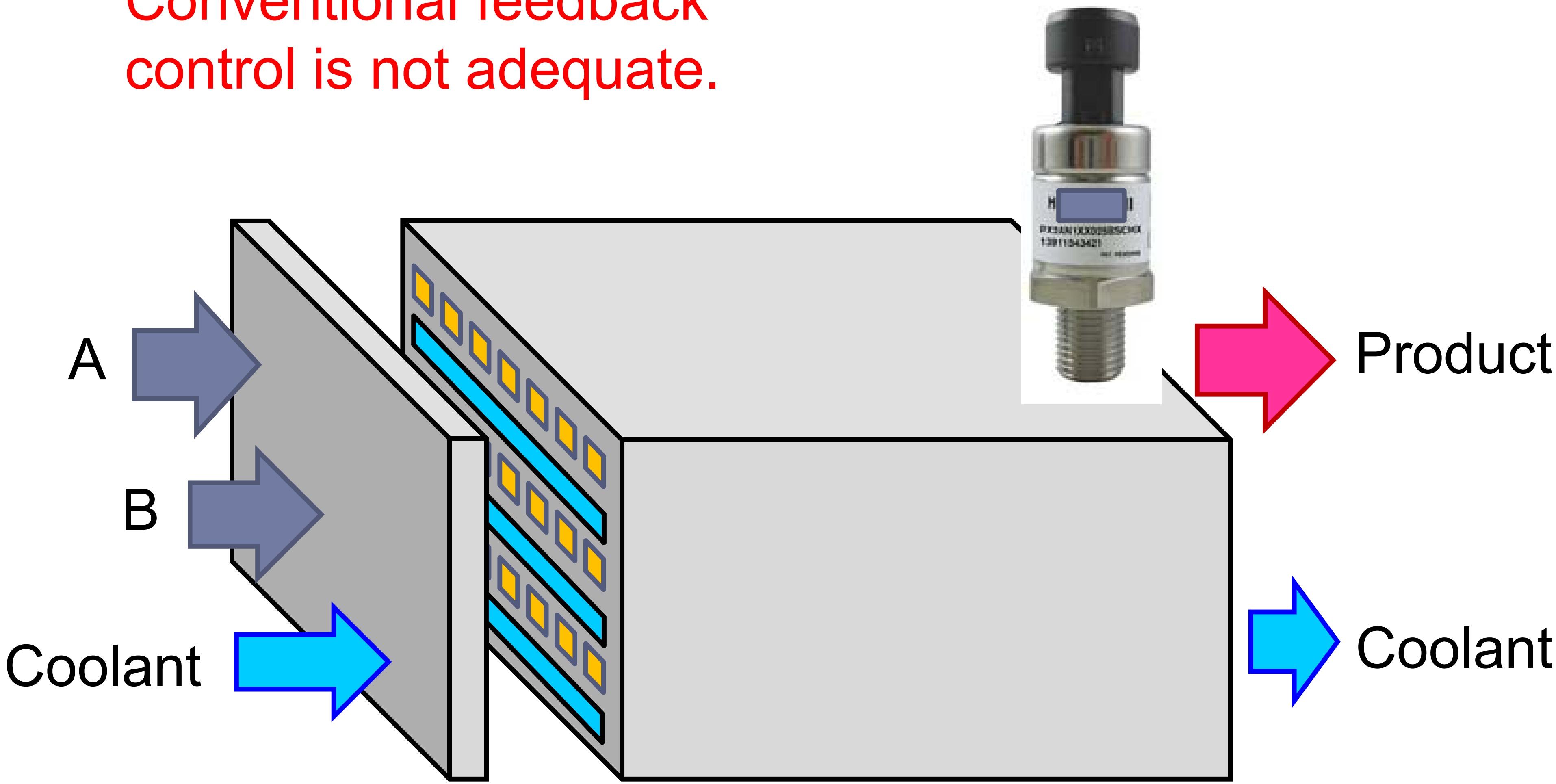
Fast, exothermic reaction



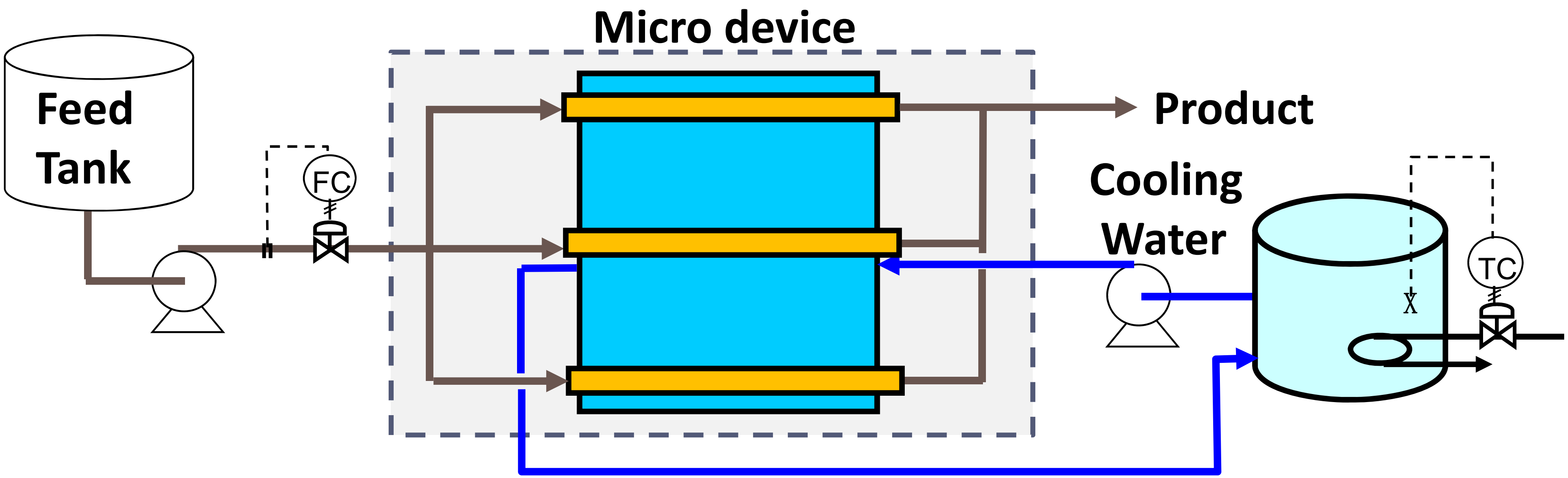
Control of Stacked Device

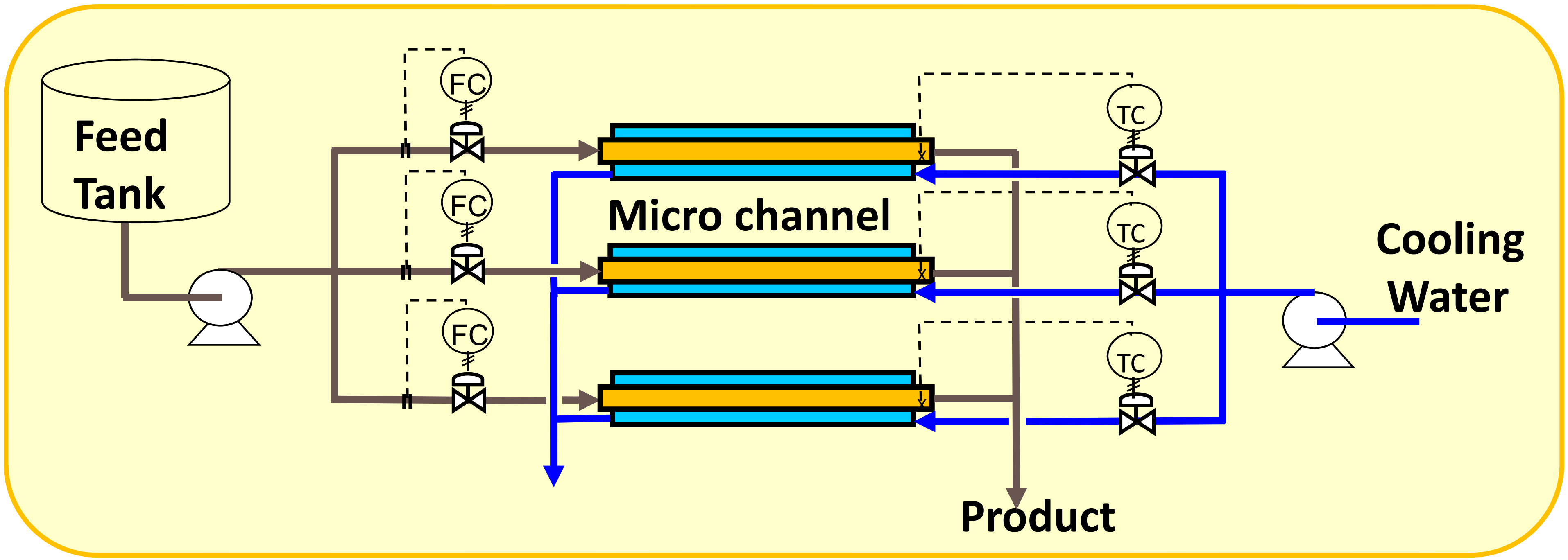
Measuring instruments and actuators cannot be installed after the device has been constructed.

Conventional feedback control is not adequate.

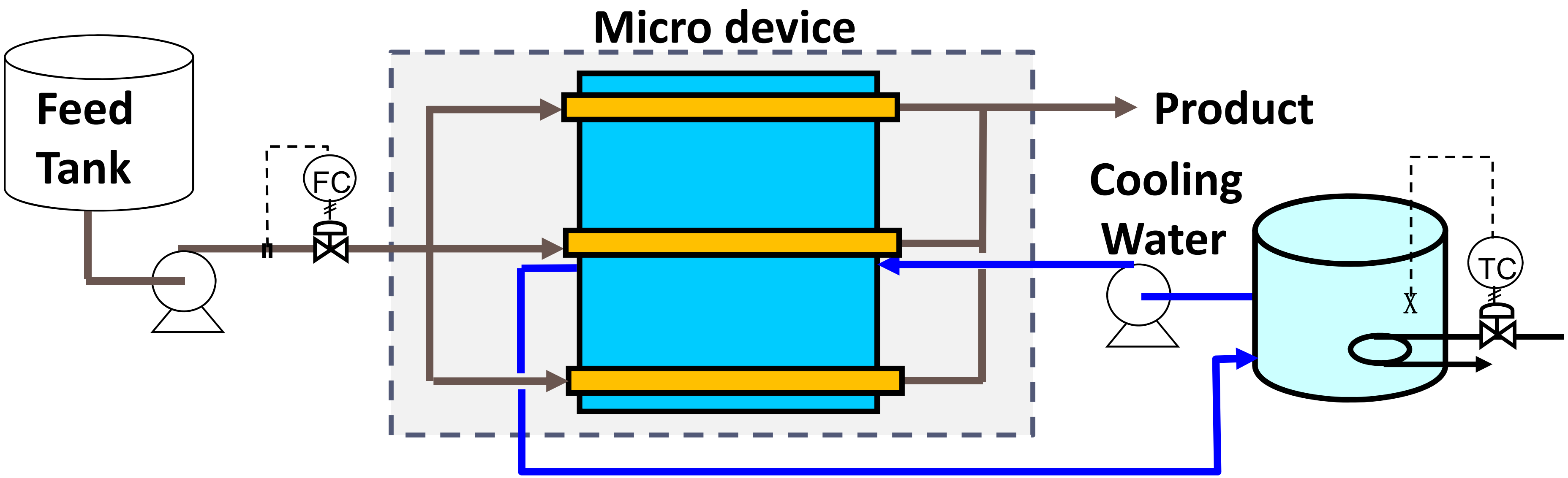


Reduction of Controllers





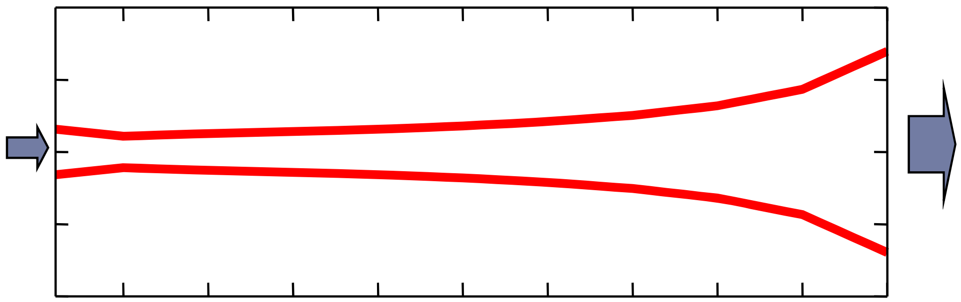
Control by Process Design



Ensure the process condition
not by control but by process design.

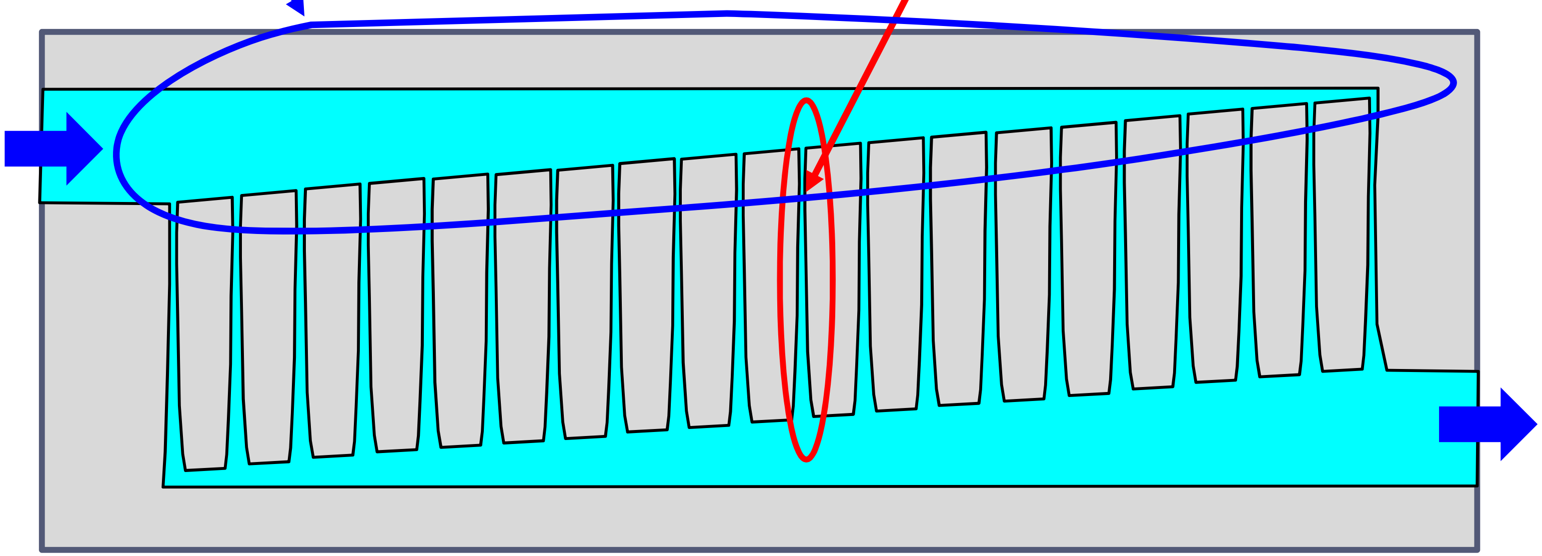
Design of Micro Device

The shape of micro channel is optimized.

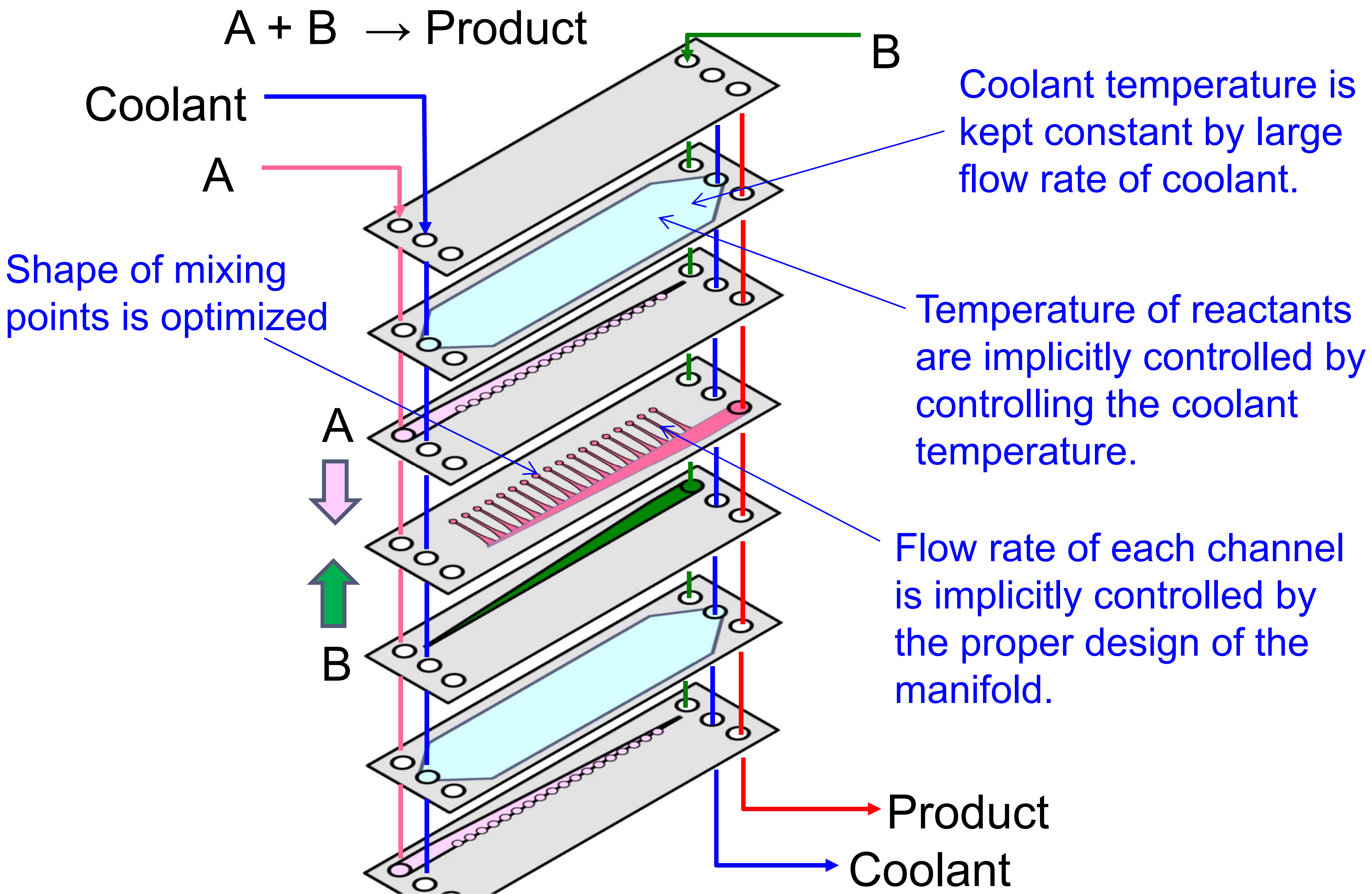


The shape of manifold is optimized so as to achieve uniform flow distribution to the channels.

Micro channel



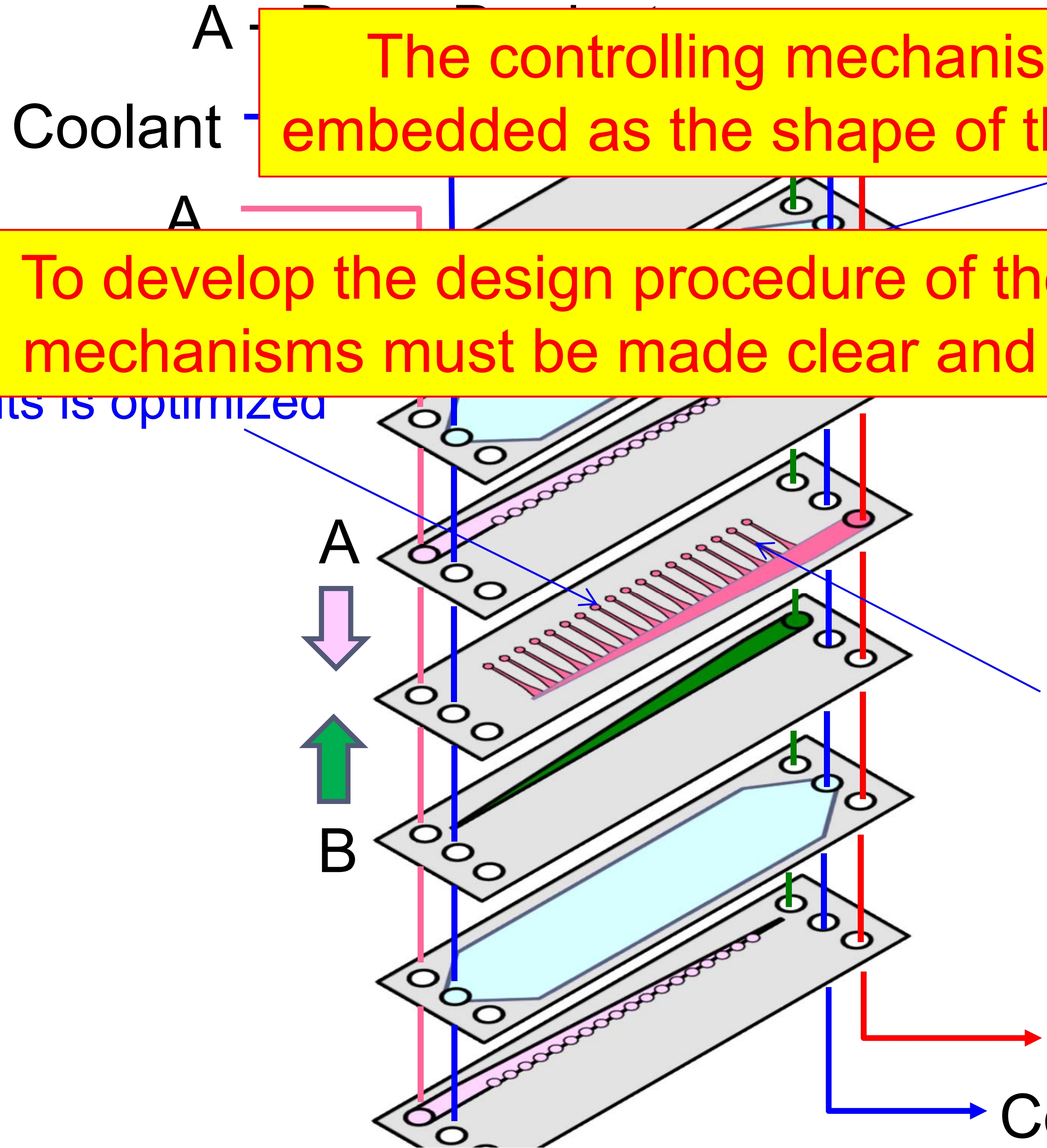
Stacked Plate Type Micro Device



Stacked Plate Type Micro Device

The controlling mechanisms are embedded as the shape of the device.

To develop the design procedure of the micro devices, these mechanisms must be made clear and included in the model.



…temperature is …stant by large flow rate of coolant

Sh… points is optimized

…emperature of reactants are implicitly controlled by controlling the coolant temperature.

Flow rate of each channel is implicitly controlled by the proper design of the manifold.

Contents

1. Why Micro Systems?
2. Feature of Design Problem of MCP
3. Contribution of PSE

Future Problems

- There are still many problems which must be solved by Process Systems Engineers.
  - Design with shape optimization
  - Design of numbering-up structure
  - Estimation of unmeasured variables
  - Simultaneous optimization of design and control problems

    :
- Microchemical plants are appropriate tools for Process Systems Engineers to verify their ideas.

- Self control mechanism/ Robust design

  Process should be robust for the unexpected disturbances.

- Reconstruction of conventional unit operations by using precise models

Verification of New Ideas

Process Systems Engineers have proposed many new design and/or control procedures.

We do not have real plants in the lab.
Real application depends on the mind of industrial engineers.

The real plant is different from the model.

We can design, construct and operate the plants by ourselves.
(ex. 3-D printer)

Your proposal is true only for the proposed model.

⇨ **Construct a plant that acts the same as the model**

There arise many unforeseen problems in the real operation.

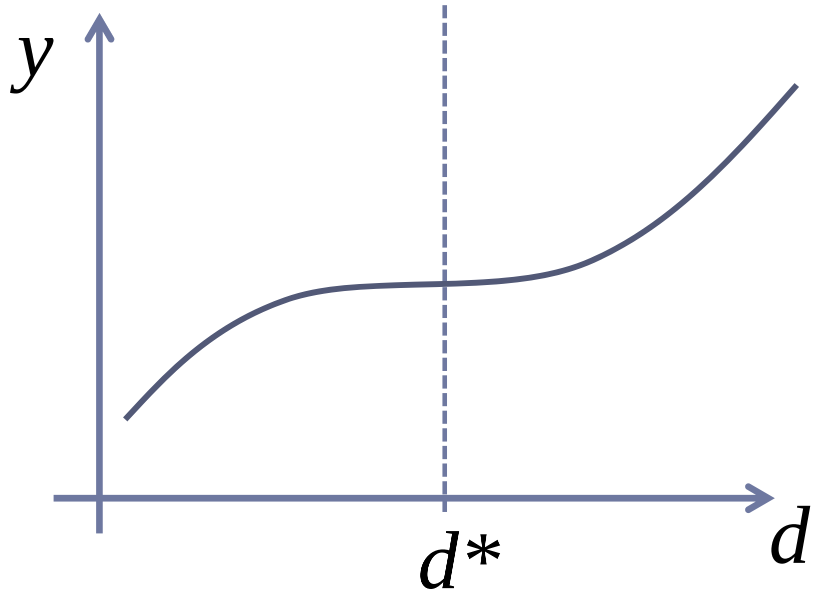
⇨ **Propose the operation that does not generate disturbances, or design the plant with enough robustness**

Self control mechanism/ Robust design

- **Positive usage of non-linear relationship**

$$y = f(x, d)$$

d: disturbance

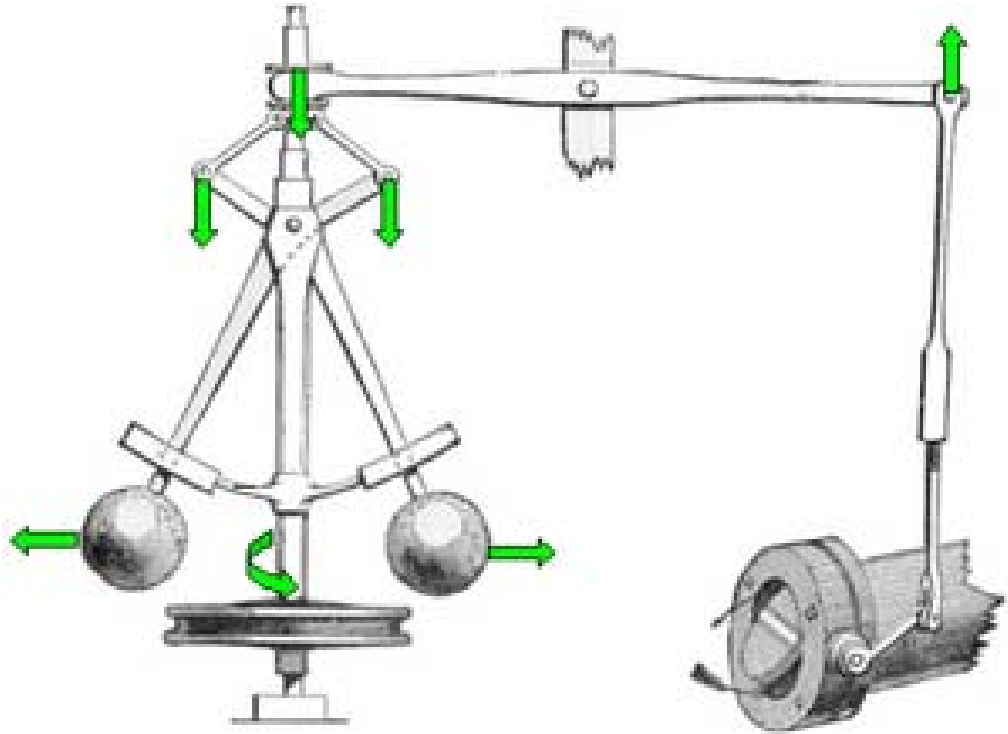


- **Embedding of feedback mechanism**

Embedding of Feedback Mechanism

Centrifugal Governor

Boulton & Watt engine of 1788

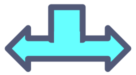
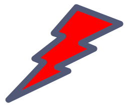
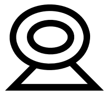


On steam engines, it regulates the admission of steam into the cylinder.

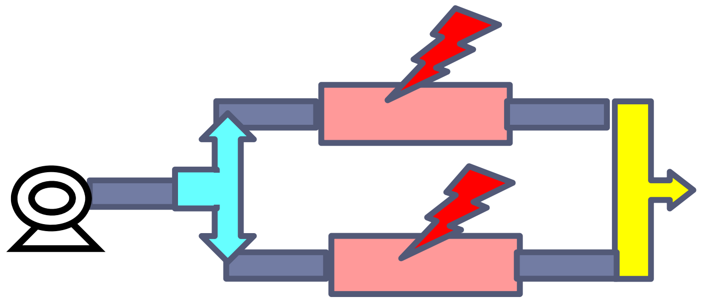
From Wikipedia

Embedding of Feedback Mechanism

Building blocks of a device

- Flow channel 
- Reactor channel 
- Splitter 
- Mixer 
- Heat supplier 
- Pump with constant flow rate
- Pump with constant pressure 

Optimal design of structure, size and shape



- Temperature sensitive channel

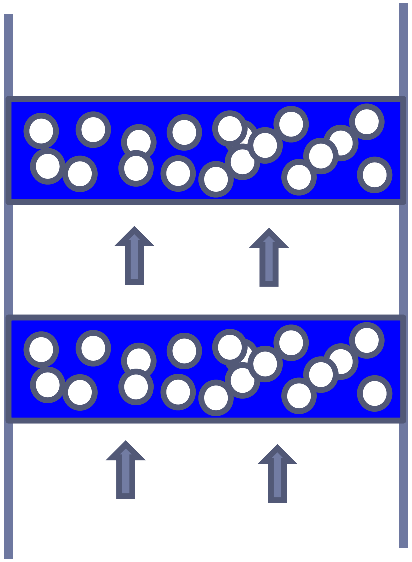
  high –> shrinking or expansion
- Pressure sensitive channel

  high –> shrinking or expansion

Superstructure based optimization (MINLP)
+
Process knowledge
+
Knowledge acquisition

Reconstruction of Conventional Unit Operations

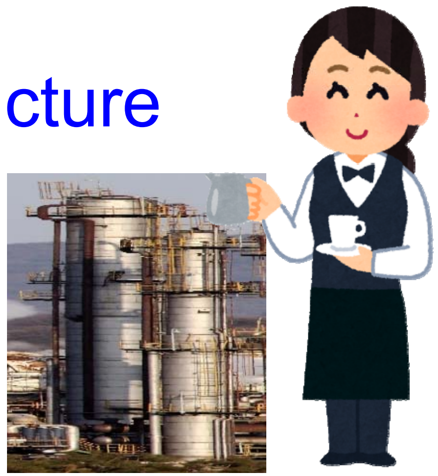
Why is the distillation column so tall?



Why does each stage need 60 to 100 cm?

Vapor space velocity = 1.0 m/s
Residence time = 0.01 sec

If we can find the structure that satisfies above conditions,



Reconstruction of Conventional Unit Operations

From Improvement to Innovation

Development of precise physical model

↓

Optimization without hardware constraints

↓

Creation of new hardware structure

Micro systems have potential
to realize this design scheme

Thank you for your attention

Katsuta Campus of Kyoto University