オープンCAEシンポジウム2012@岐阜

熱物質移動を含むプロセスへのオープンCAEの活用

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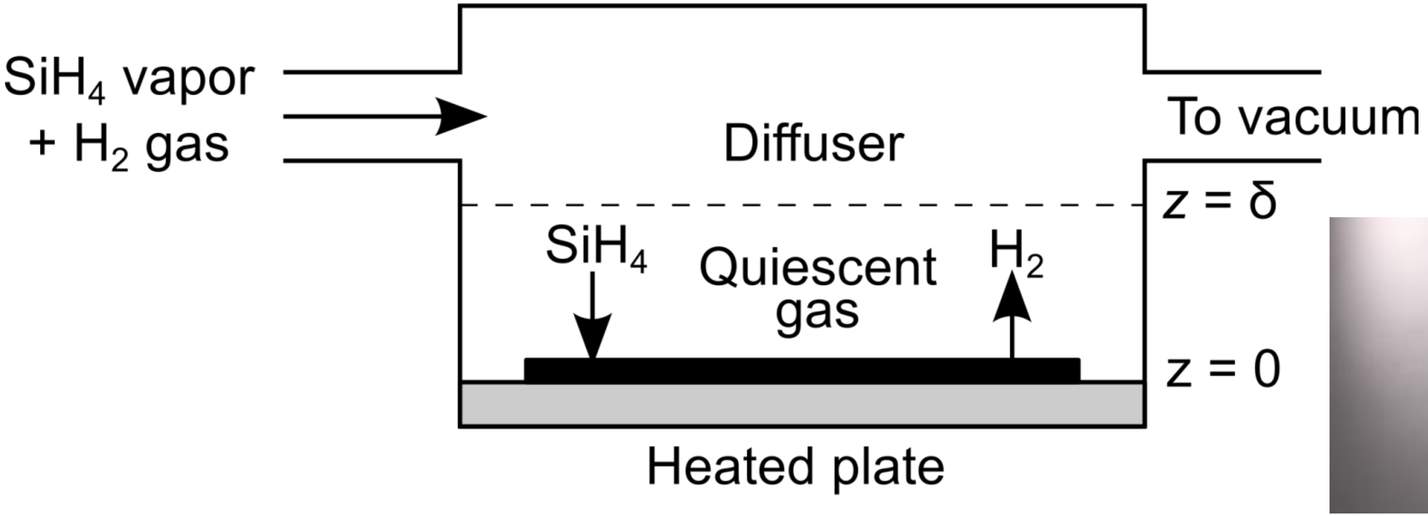
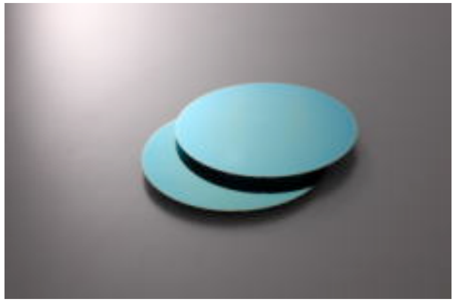
Chemical engineering process

Ex. Chemical Vapor Deposition (CVD)

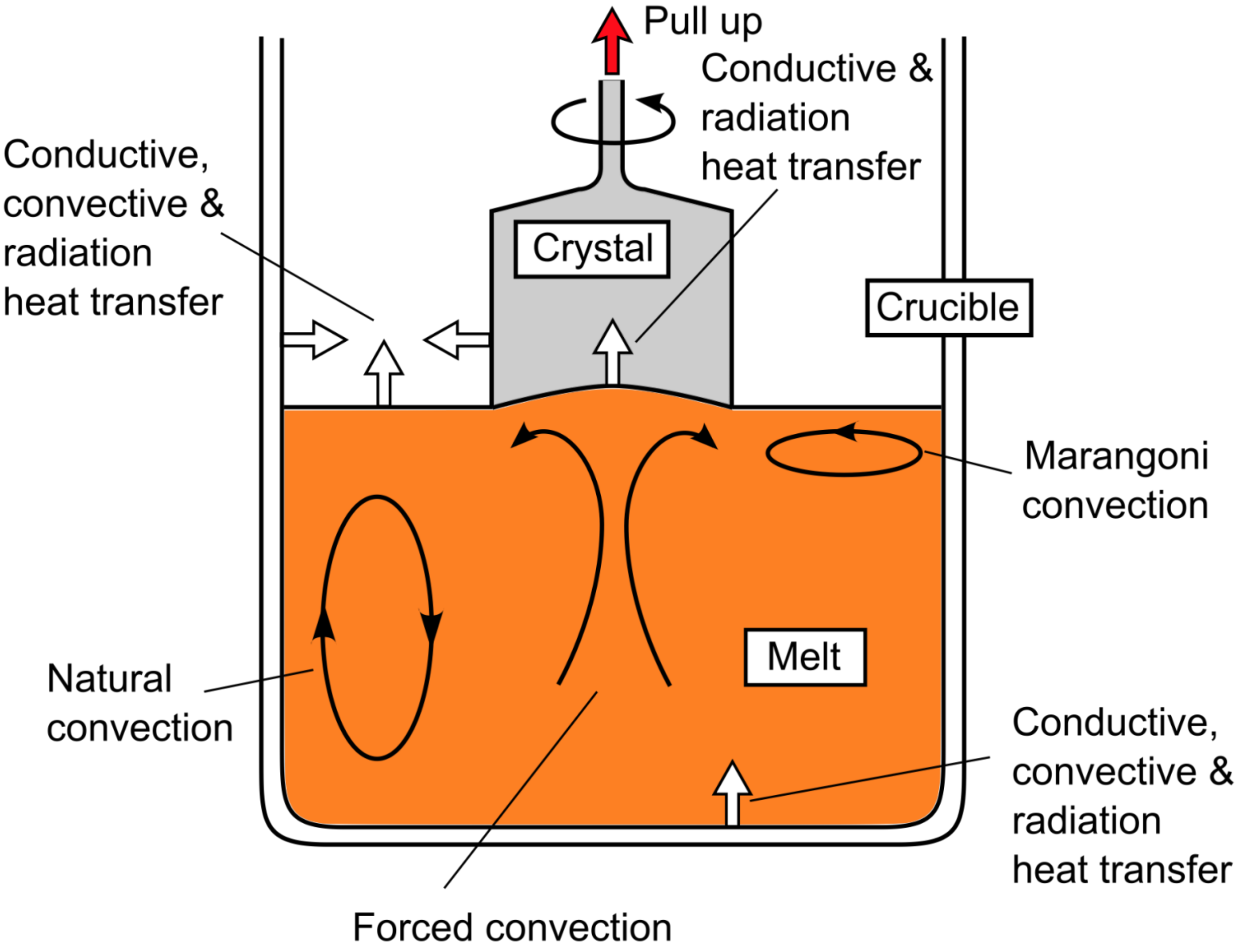


$$SiH_4(g) \rightarrow Si(s) + 2H_2(g)$$



Heat, Mass and momentum transfer

Transport phenomena in melt



Governing equations in melt

- Navier-Stokes eq.

$$\underline{\frac{\partial \mathbf{u}}{\partial t}} + \underline{\mathbf{u}\cdot \nabla \mathbf{u}} = -\frac{1}{\rho}\nabla P + \underline{\nu \nabla^2 \mathbf{u}} + \mathbf{F}$$

- Energy eq.

$$\underline{\frac{\partial T}{\partial t}} + \underline{\mathbf{u}\cdot \nabla T} = \underline{\alpha \nabla^2 T}$$

- Diffusion eq.

$$\underline{\frac{\partial C}{\partial t}} + \underline{\mathbf{u}\cdot \nabla C} = \underline{D \nabla^2 C}$$

$\mathbf{u}$: vector
T: scalar
C: scalar

Common operator:
Gradient, Divergence, Laplacian, Time Advancement

Advantage of open source

- OpenFOAM
  - Object Oriented Programming

```
grad(T)
grad(U)
```

Operator overload
Class module

↓

Easy extension

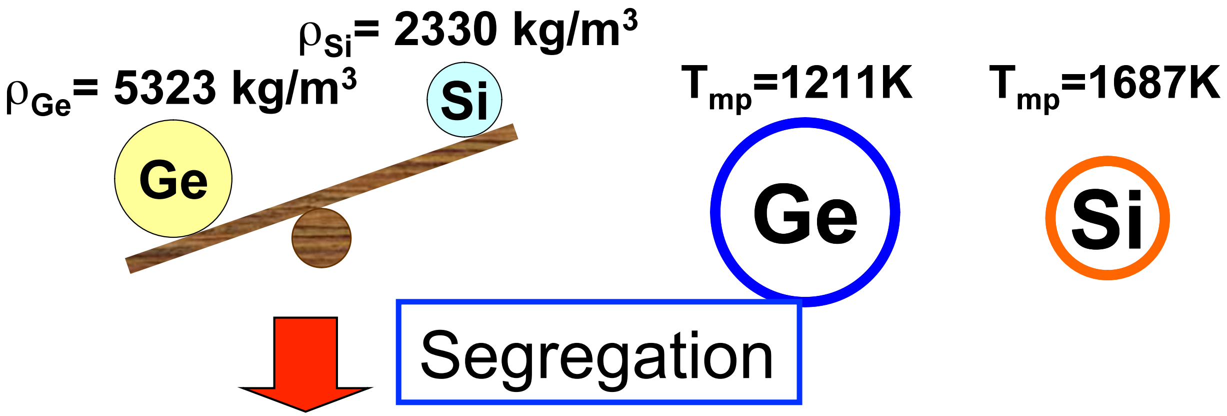
- Fortran code
  - Procedural Programming

```
call grad(T,dTdx,dTdy,dTdz)
call grad(u,dudx,dudy,dudz)
call grad(v,dvdx,dvdy,dvdz)
call grad(w,dwdx,dwdv,dwdz)
```

Mixture of scalar, vector and tensor

Crystal growth of compound semiconductor

- Silicon germanium (SiGe)
  - (Si_xGe_{1-x})
  - High performance, high efficiency
  - Lattice mismatch in Si+SiGe
- Property of SiGe



ρ_{Si}= 2330 kg/m^3

ρ_{Ge}= 5323 kg/m^3

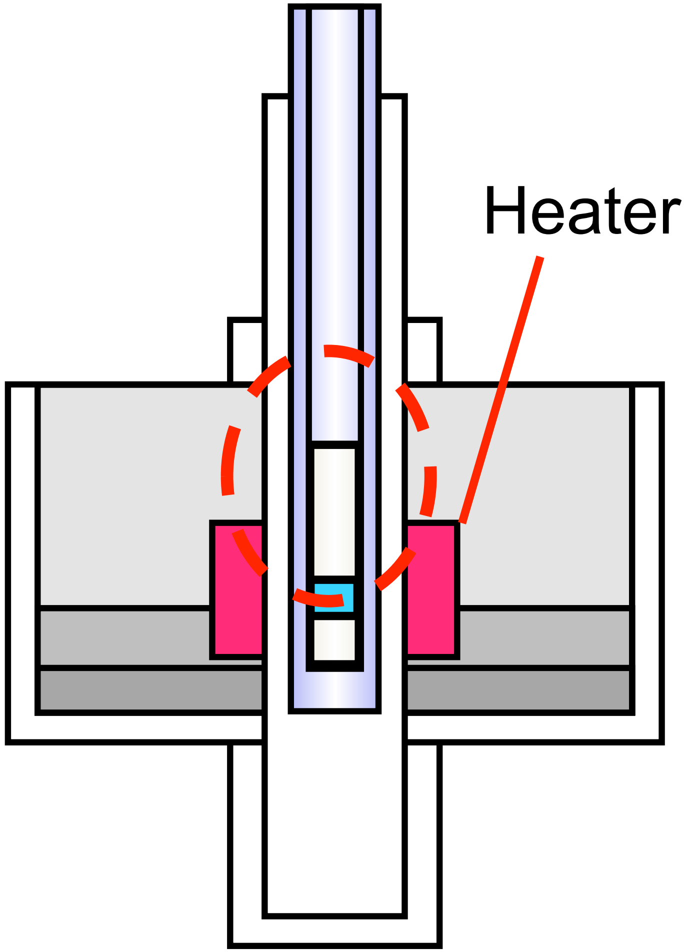
T_{mp}=1211K

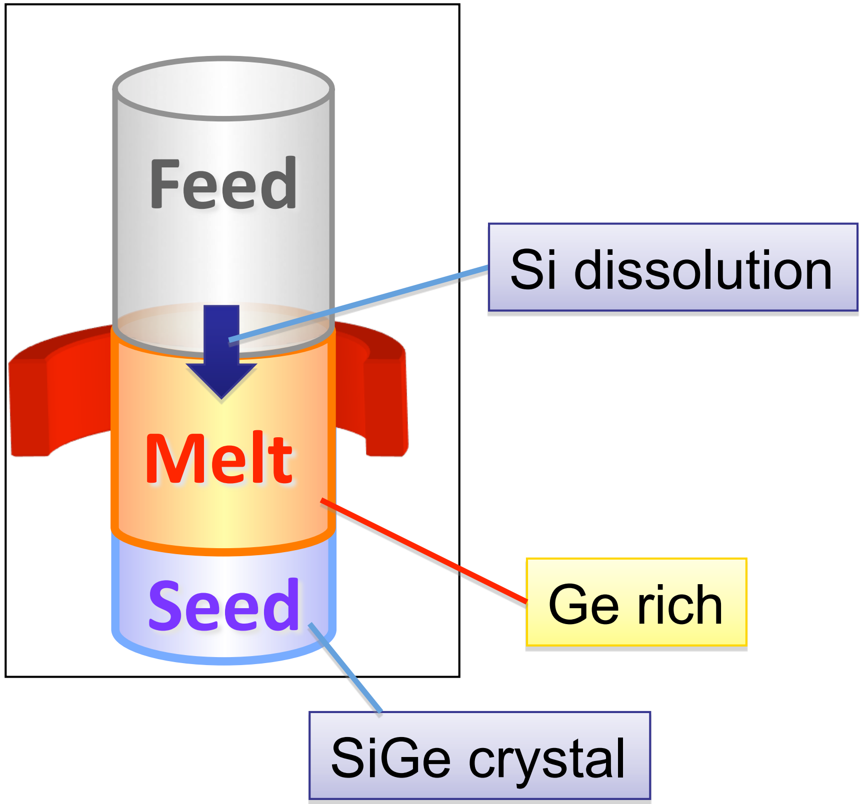
T_{mp}=1687K

Segregation

Use of solution growth

Traveling Heater Method (THM)





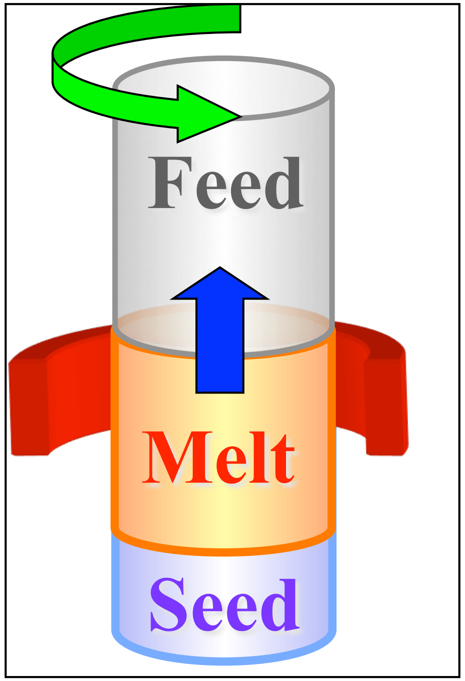
Melt convection with heat and mass transfers

Objective

- Convection control in THM
  - Magnetic field
  - Crucible rotation

OpenFOAM

- Convection suppression effect with external forces
- Operating condition for high quality crystal
  - Si concentration near growth interface



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Governing equations in melt

- Navier-Stokes eq.

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\frac{1}{\rho}\nabla P + \nu\nabla^2\mathbf{u} + \underline{\mathbf{S}} + \underline{\mathbf{F}}$$

$$\underline{\mathbf{S} = \left(\beta_T g\left(T - T_0\right) - \beta_C g\left(C - C_0\right)\right)\mathbf{e}_Z} \qquad \underline{\mathbf{F} = \mathbf{J}\times\mathbf{B}}$$

- Induction eq. of magnetic field

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla\cdot\left(\mathbf{u}\times\mathbf{B} - \mathbf{B}\times\mathbf{u}\right) - \nabla\cdot\frac{1}{\sigma\mu}\nabla\mathbf{B} = 0$$

- Energy eq.

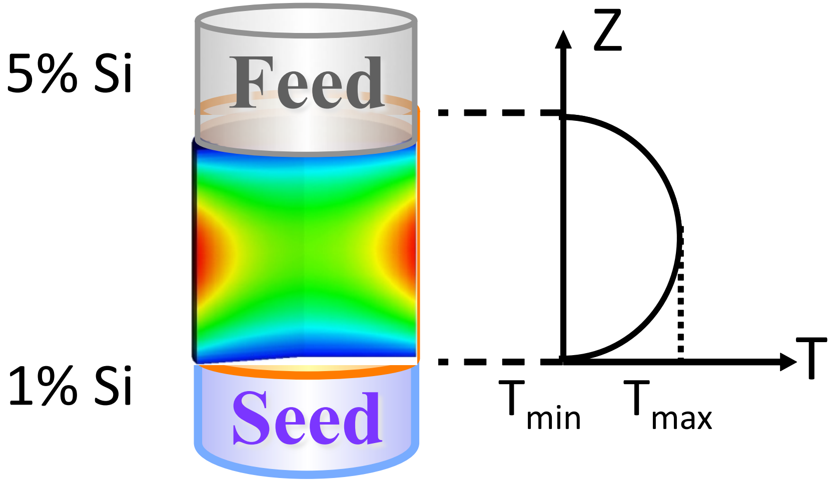
$$\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T = \alpha\nabla^2 T$$

- Diffusion eq.

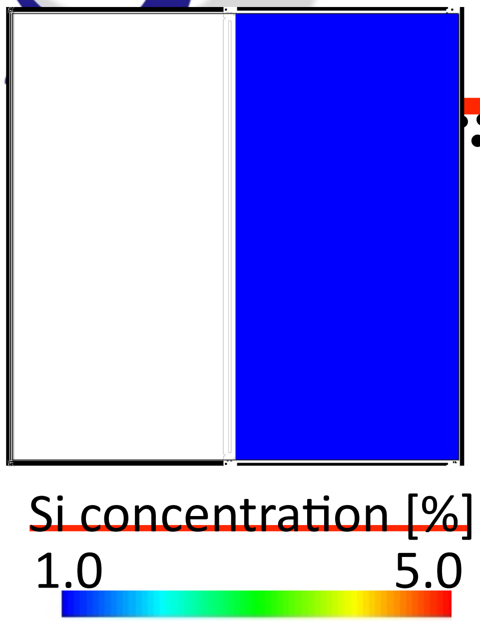
$$\frac{\partial C}{\partial t} + \mathbf{u}\cdot\nabla C = D\nabla^2 C$$

Boundary condition

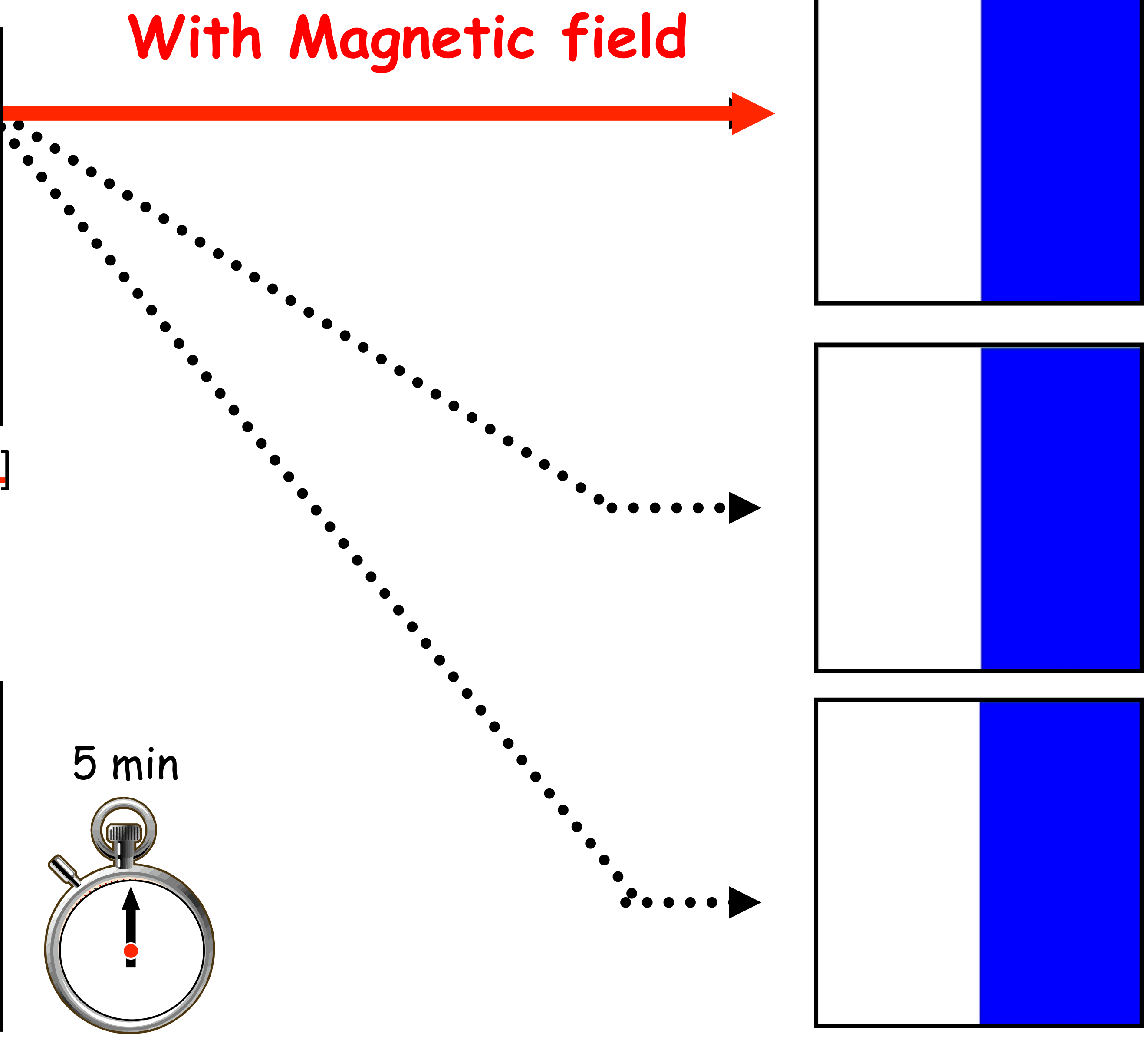
- Velocity: no-slip condition, rotating wall velocity
- Magnetic field： static vertical
- Temperature and concentration:



- Not considered: moving boundary of crystal-melt surface, heater movement

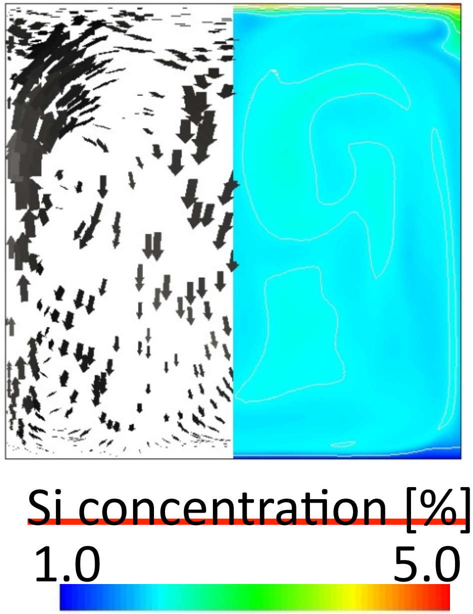


No control

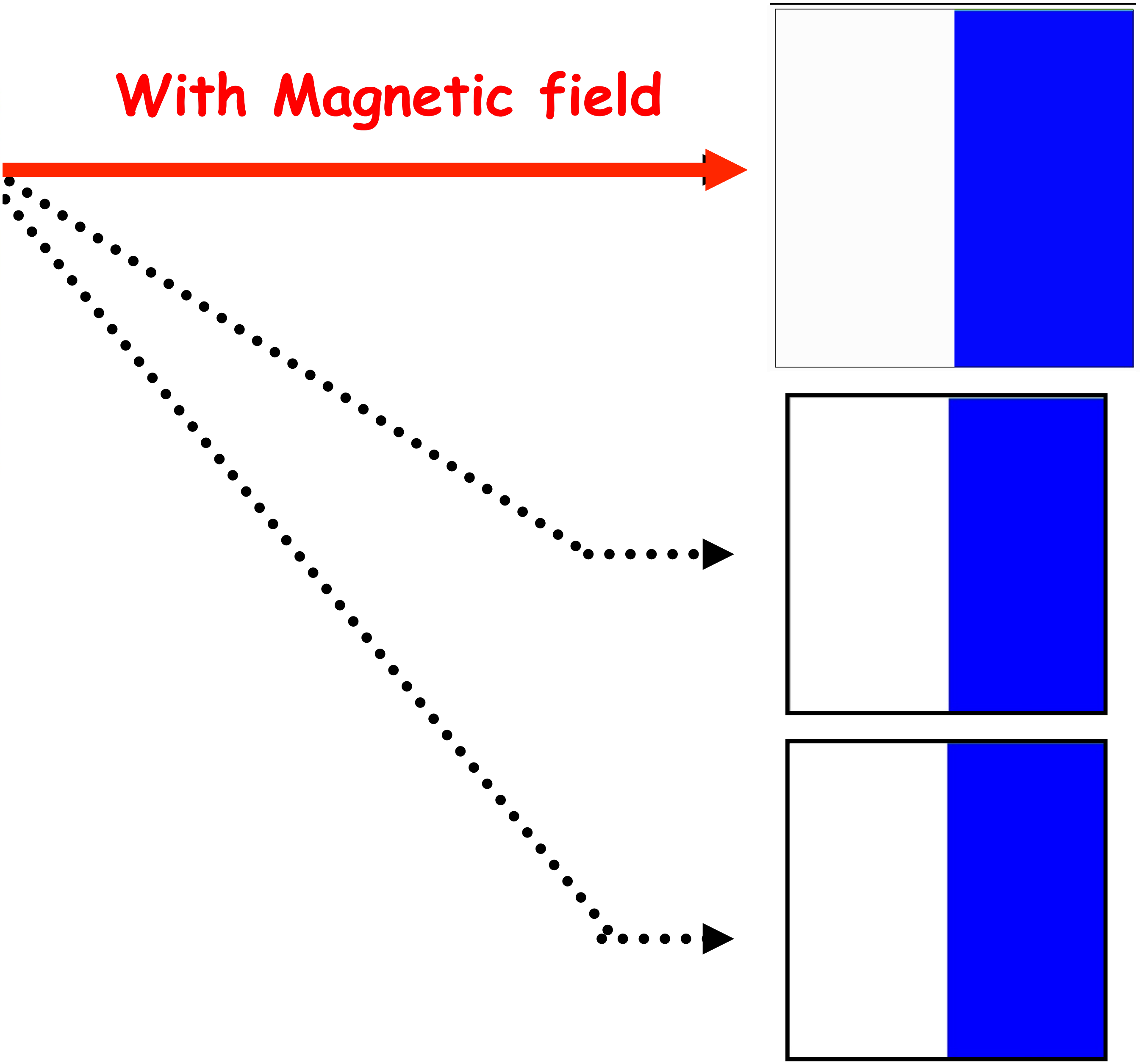


	M.F.	Rot.
Case1	×	×
Case2	○	×
Case3	×	○
Case4	○	○

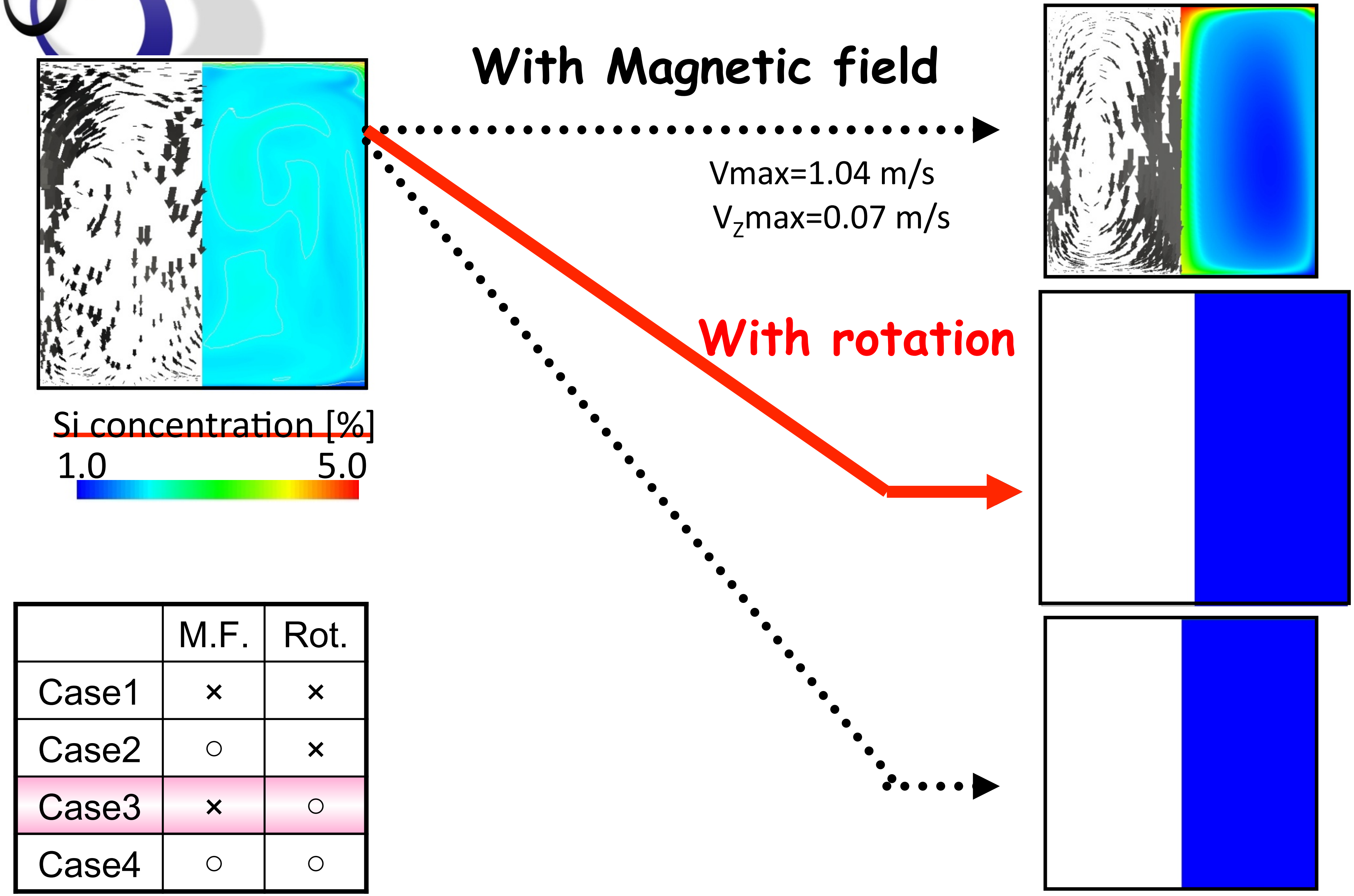
5 min



No control



	M.F.	Rot.
Case1	×	×
Case2	○	×
Case3	×	○
Case4	○	○



With Magnetic field

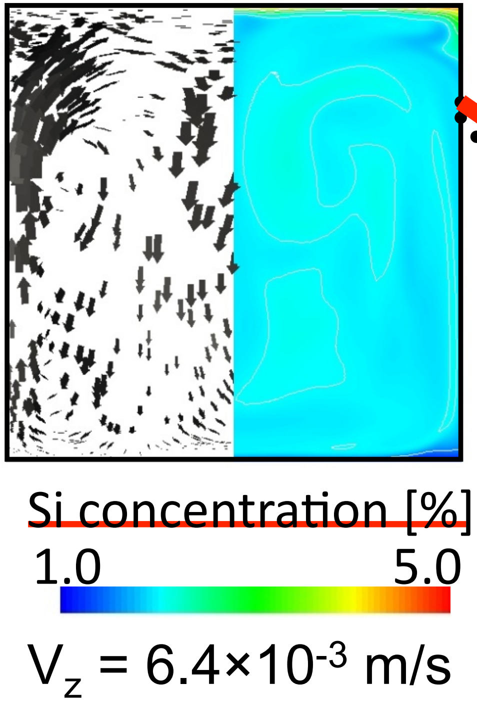
Vmax=1.04 m/s

$V_z$max=0.07 m/s

With rotation

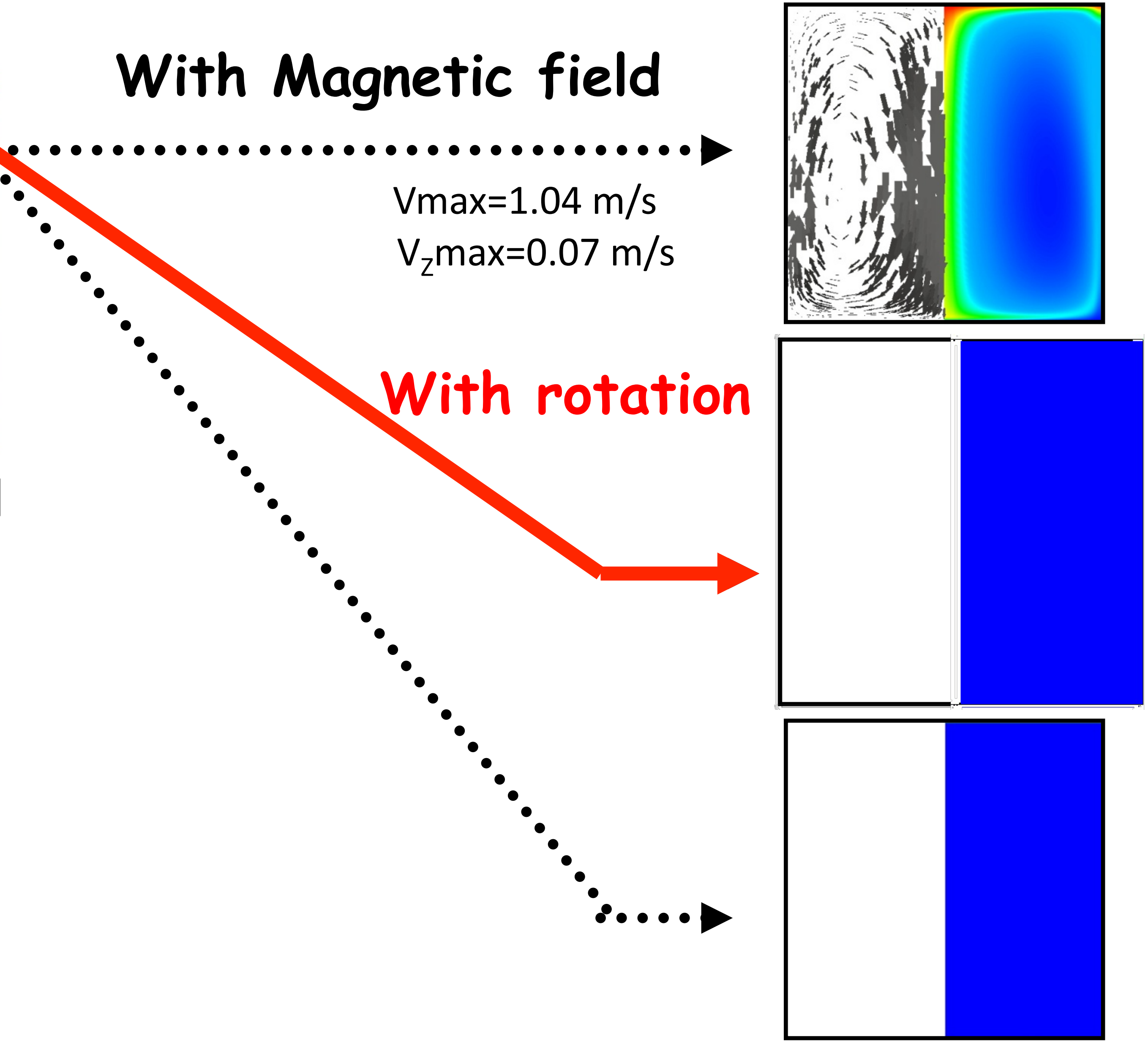
Si concentration [%]

	M.F.	Rot.
Case1	×	×
Case2	○	×
Case3	×	○
Case4	○	○



$V_z = 6.4\times10^{-3}$ m/s

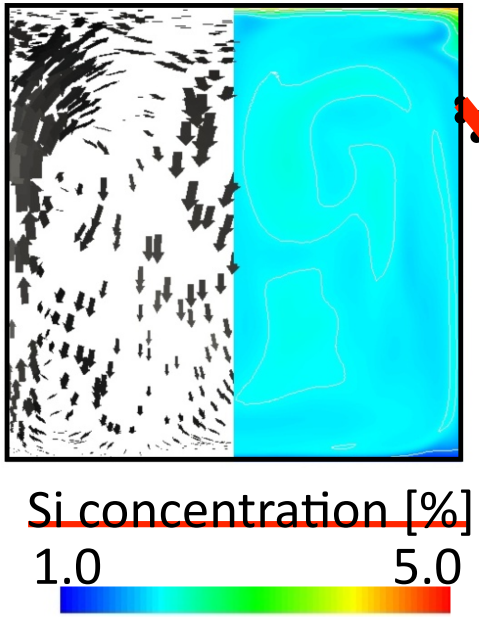
	M.F.	Rot.
Case1	×	×
Case2	○	×
Case3	×	○
Case4	○	○

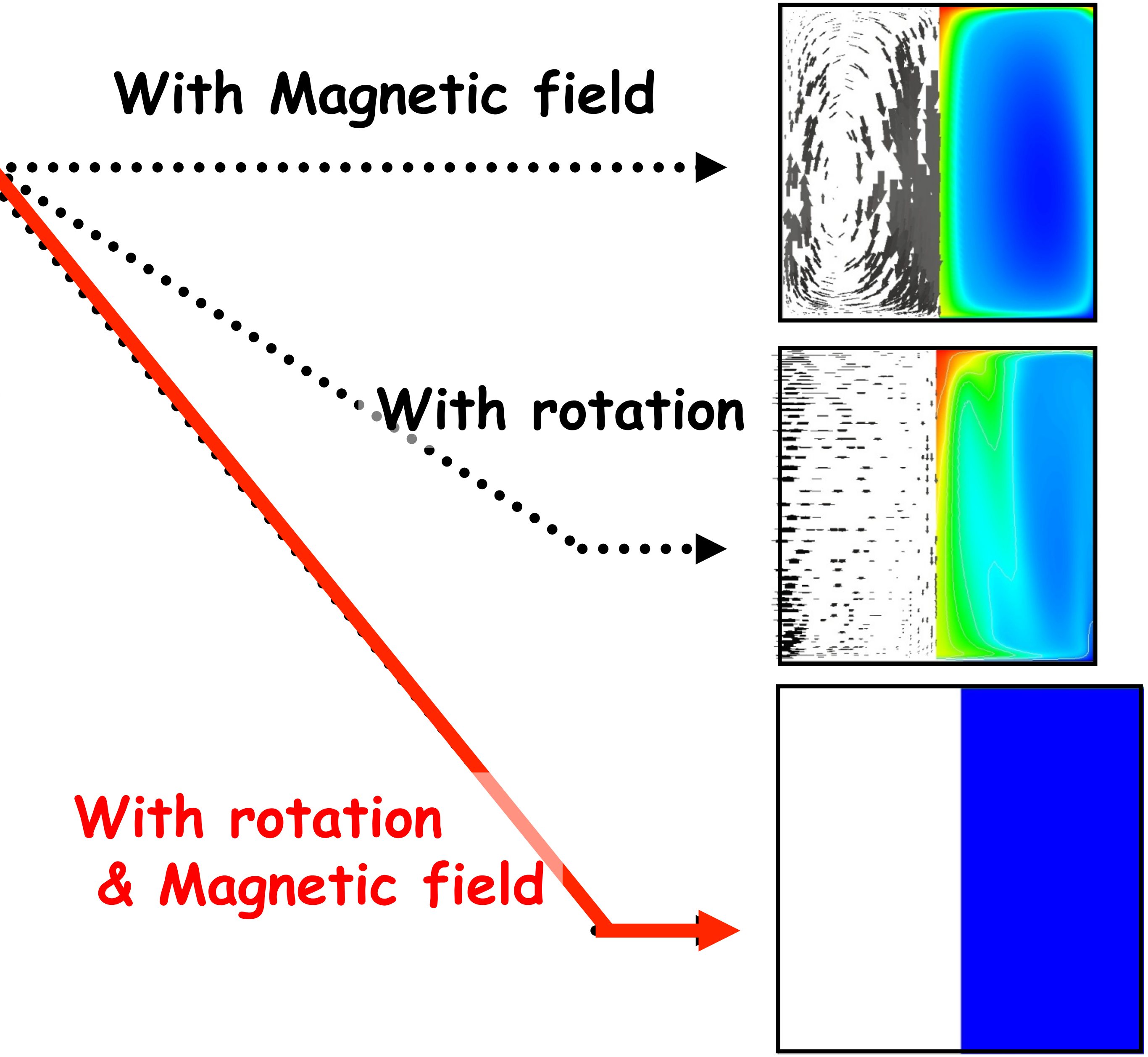


With Magnetic field

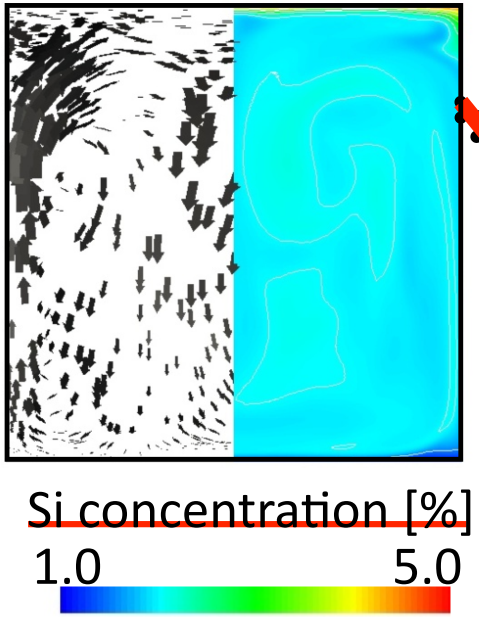
Vmax=1.04 m/s
$V_z$max=0.07 m/s

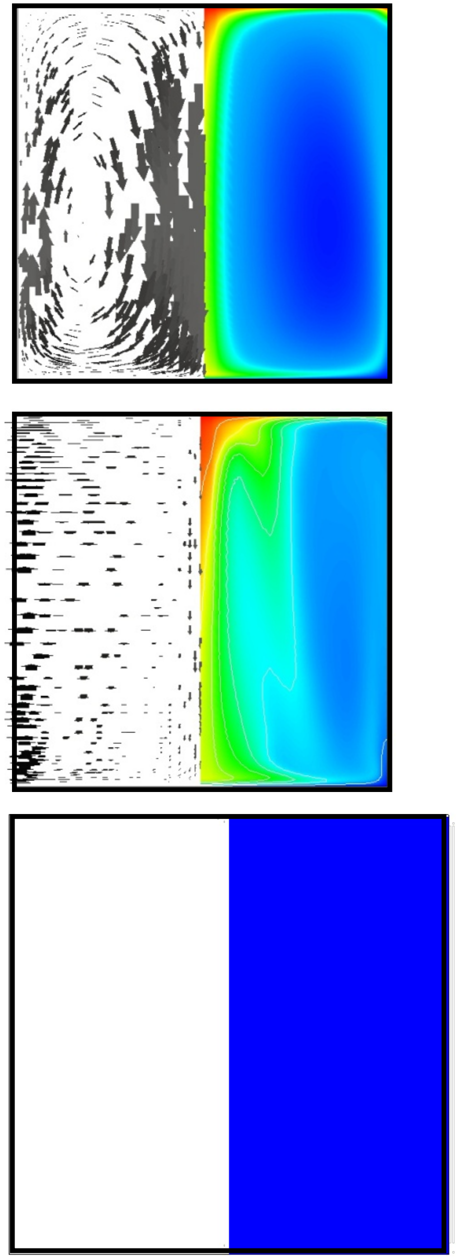
With rotation





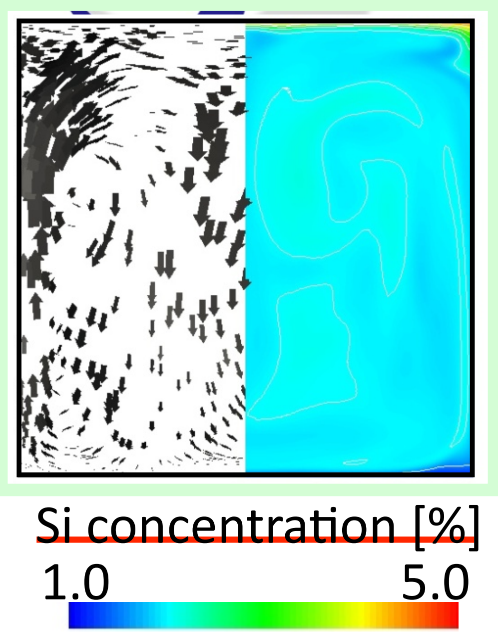
	M.F.	Rot.
Case1	×	×
Case2	○	×
Case3	×	○
Case4	○	○

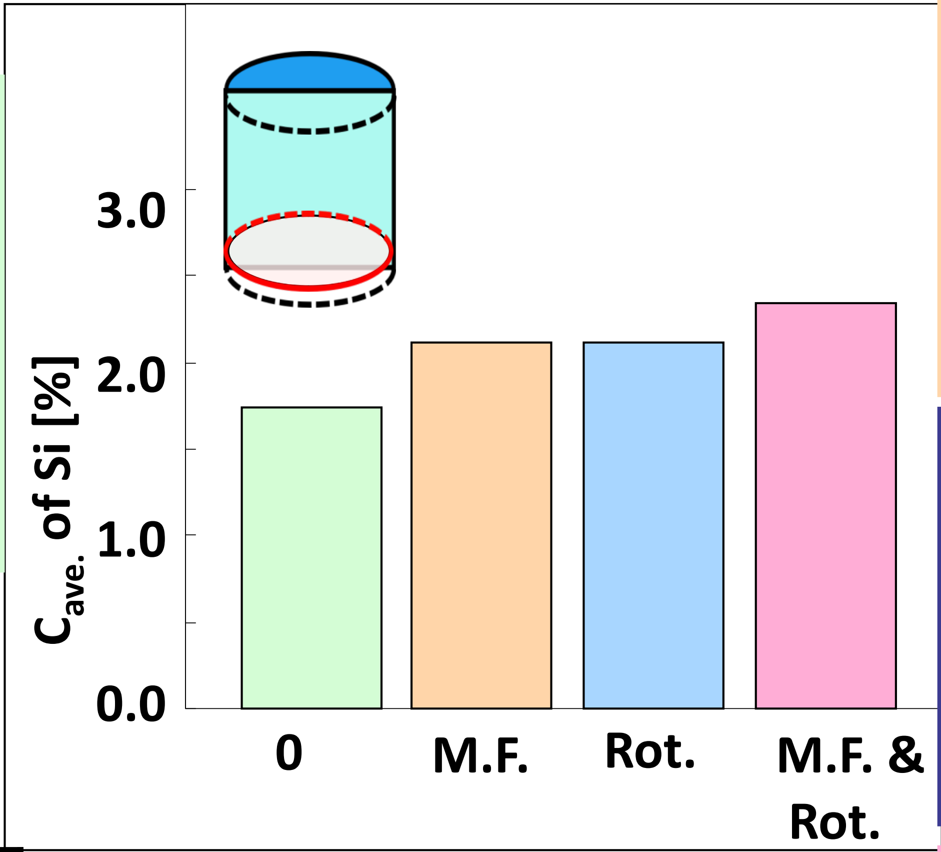


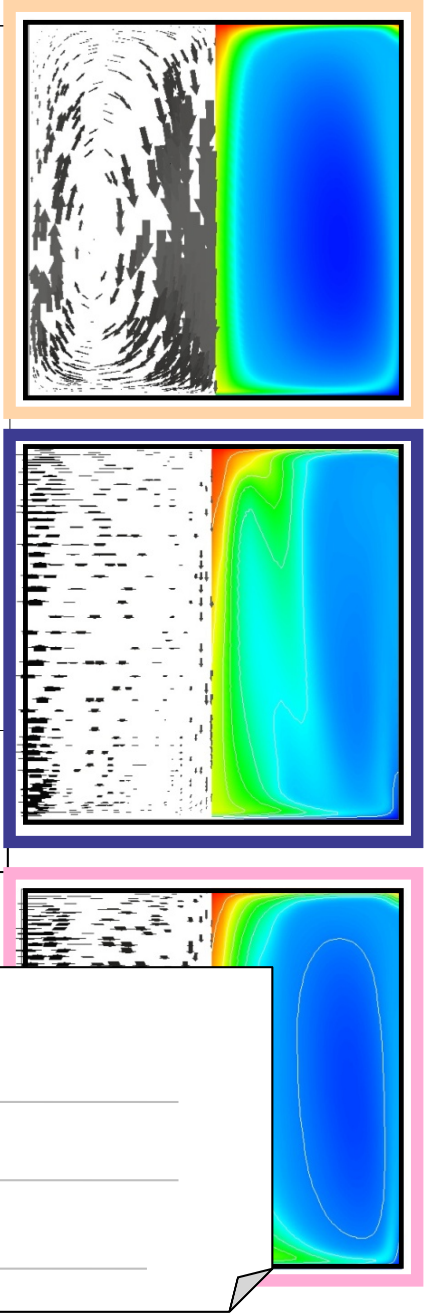


With rotation & Magnetic field

	M.F.	Rot.
Case1	×	×
Case2	○	×
Case3	×	○
Case4	○	○



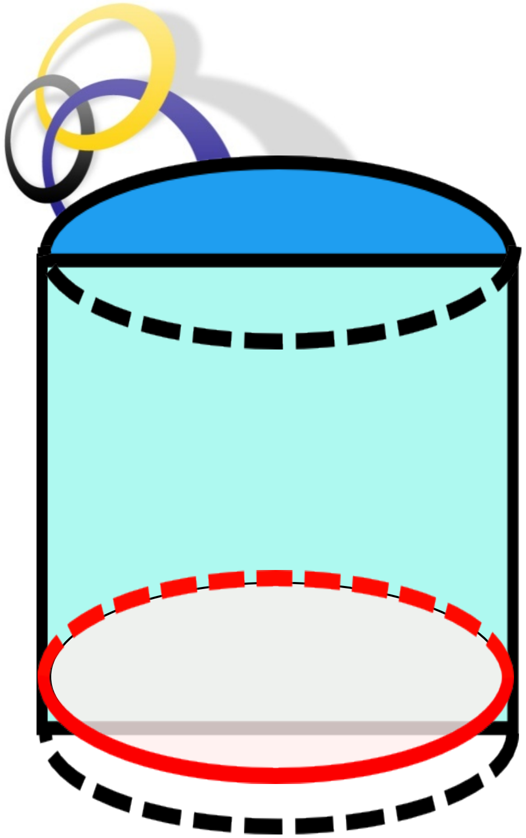


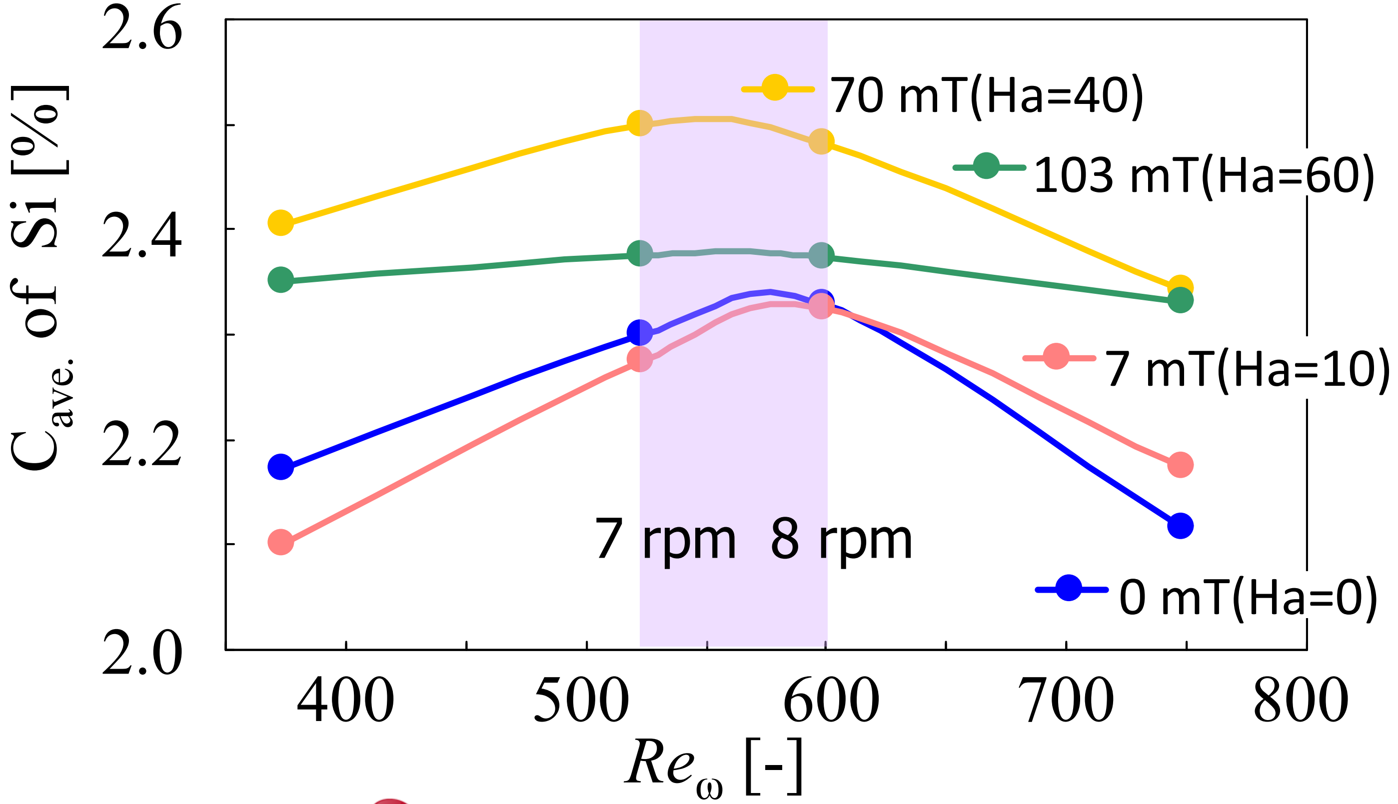


	M.F.	Rot.
Case		
Case		
Case		
Case		

★ ***Combination of M.F. and rotation***

Rich Si near growth interface





Best

★ ***Combination of M.F. and rotation***

7-8 rpm & around 70mT(Ha=40)

Rich Si near growth interface

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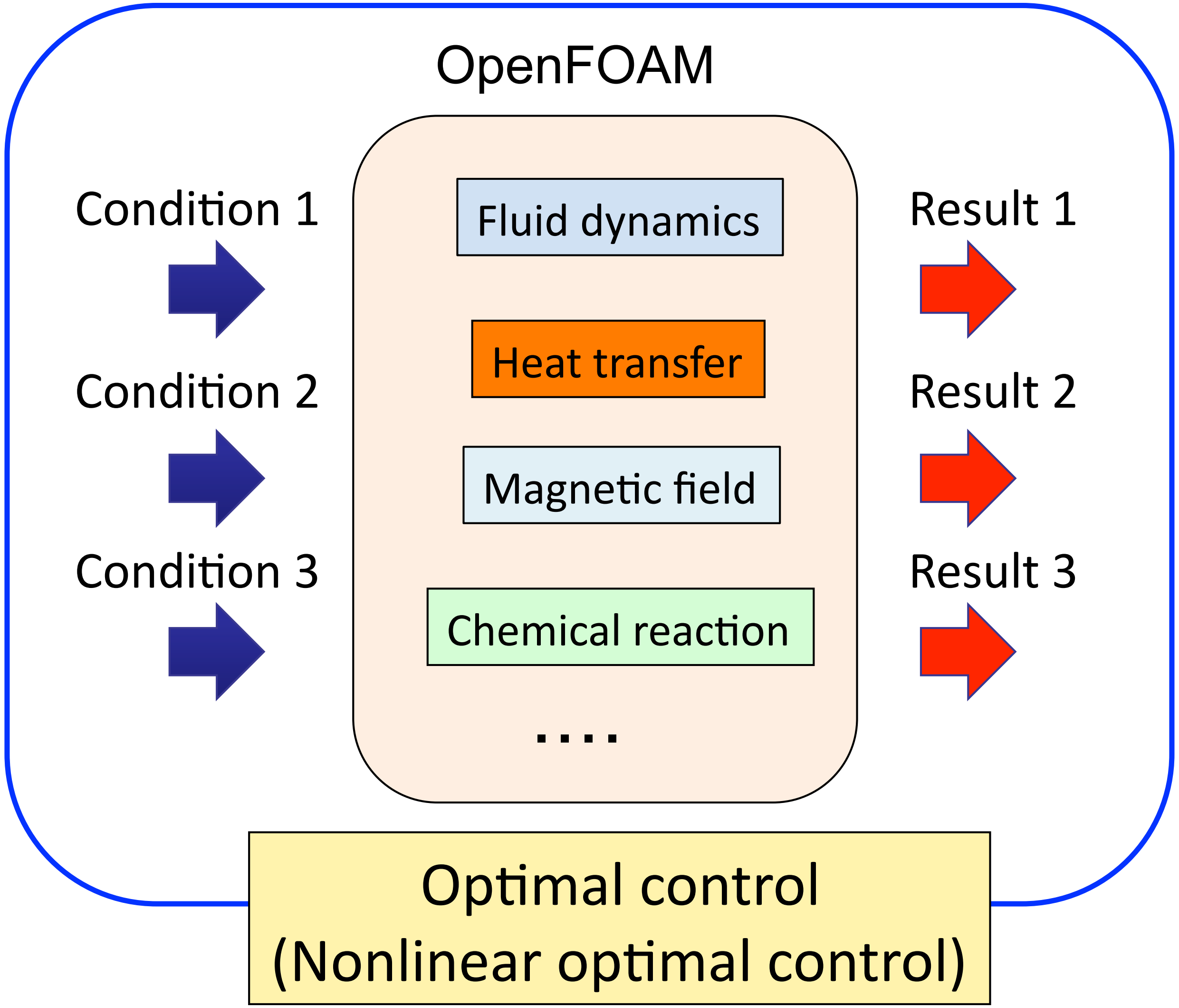
Toward smart control



OpenFOAM

Condition 1

Condition 2

Condition 3

Fluid dynamics

Heat transfer

Magnetic field

Chemical reaction

....

Result 1

Result 2

Result 3

Optimal control
(Nonlinear optimal control)

First step for smart control: Adjoint method

Adjoint method formulation for ducted flow

- Adjoint N-S equations:

$$-2\mathrm{D}(\mathbf{u})\mathbf{v} = -\nabla q + \nabla\cdot(2\nu\mathrm{D}(\mathbf{u})) - \alpha\mathbf{u}$$

$$\nabla\cdot\mathbf{u} = 0$$

- Adjoint BCs for the wall and inlet:

$$\mathbf{u}_t = 0, \quad u_n = -\frac{\partial J_\Gamma}{\partial p}$$

$$\mathbf{n}\cdot\nabla q = 0$$

- Adjoint BCs for the outlet:

$$q = \mathbf{u}\cdot\mathbf{v} + u_n v_n + \nu(\mathbf{n}\cdot\nabla)u_n + \frac{\partial J_\Gamma}{\partial v_n}$$

$$0 = v_n\mathbf{u}_t + \nu(\mathbf{n}\cdot\nabla)\mathbf{u}_t + \frac{\partial J_\Gamma}{\partial \mathbf{v}_t}$$

Ex. 1: Dissipated power

Cost function:

$$J := -\int_\Gamma d\Gamma \left(p + \frac{1}{2} v^2 \right) \mathbf{v}\cdot \mathbf{n}$$

$$J_\Omega = 0, \quad J_\Gamma = -\left(p + \frac{1}{2} v^2 \right) \mathbf{v}\cdot \mathbf{n}$$

Derivatives for BCs:

$$\frac{\partial J_\Gamma}{\partial p} = -\mathbf{v}\cdot \mathbf{n},$$

$$\frac{\partial J_\Gamma}{\partial \mathbf{v}} = -\left(p + \frac{1}{2} v^2 \right) \mathbf{n} - (\mathbf{v}\cdot \mathbf{n})\mathbf{v}$$

Adjoint BCs for the wall and inlet:

$\mathbf{u}_t = 0$ at wall

$u_n = \begin{cases} 0 \\ v_n \end{cases}$ at inlet

Adjoint BCs for the outlet:

$$q = \mathbf{u}\cdot \mathbf{v} + u_n v_n + \nu(\mathbf{n}\cdot \nabla) u_n - \frac{1}{2} v^2 - v_n^2$$

$$0 = v_n(\mathbf{u}_t - \mathbf{v}_t) + \nu(\mathbf{n}\cdot \nabla)\mathbf{u}_t$$

adjointShapeOptimization.C

```
// Adjoint Pressure-velocity SIMPLE corrector
    {
        // Adjoint Momentum predictor

        volVectorField adjointTransposeConvection((fvc::grad(Ua) & U));

        zeroCells(adjointTransposeConvection, inletCells);

        tmp<fvVectorMatrix> UaEqn
        (
            fvm::div(-phi, Ua)
          - adjointTransposeConvection
          + turbulence->divDevReff(Ua)
          + fvm::Sp(alpha, Ua)
        );
```

$\nabla\mathbf{u}\cdot\mathbf{v}$

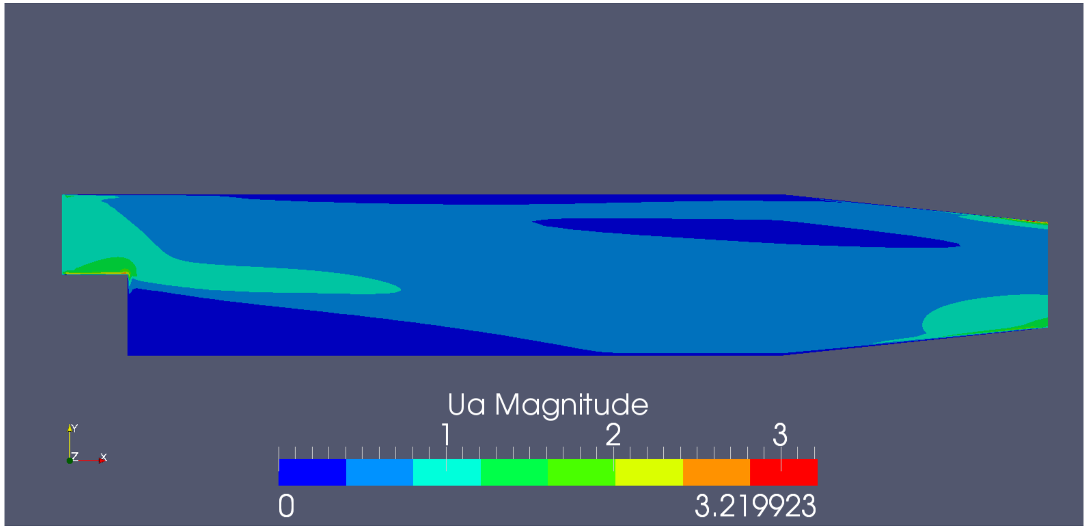
$$\nabla\cdot(-\phi\mathbf{u})$$

$$-\nabla\mathbf{u}\cdot\mathbf{v}$$

$$-\nabla\cdot(2\nu D(\mathbf{u}))$$

$$+\alpha\mathbf{u}$$

Result: adjoint velocity



Summary

- The simulation including heat, mass and momentum transfers is carried out by using OpenFOAM.
- OpenFOAM is suitable for multi-physics problem.
- Simulation code for optimization is now developed.