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Virtual solid cell for mimicking porous media in Direct Simulation Monte Carlo method

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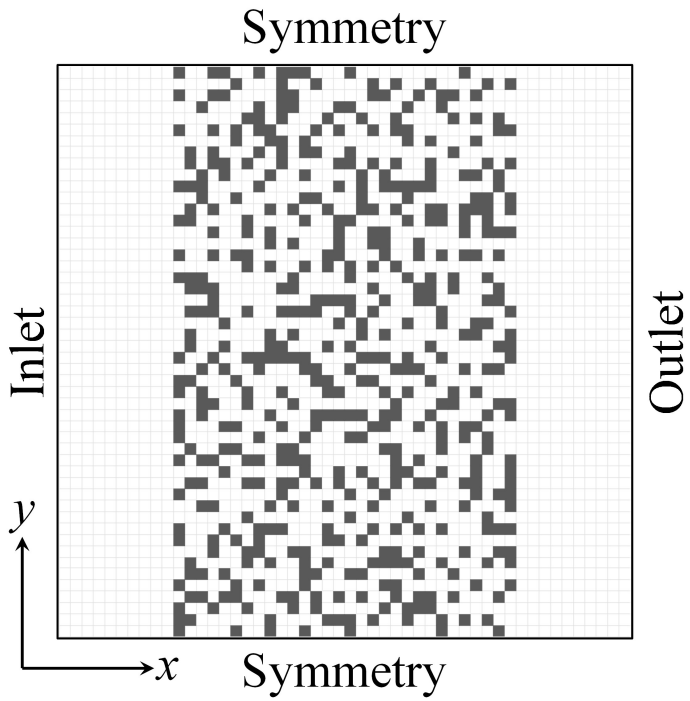
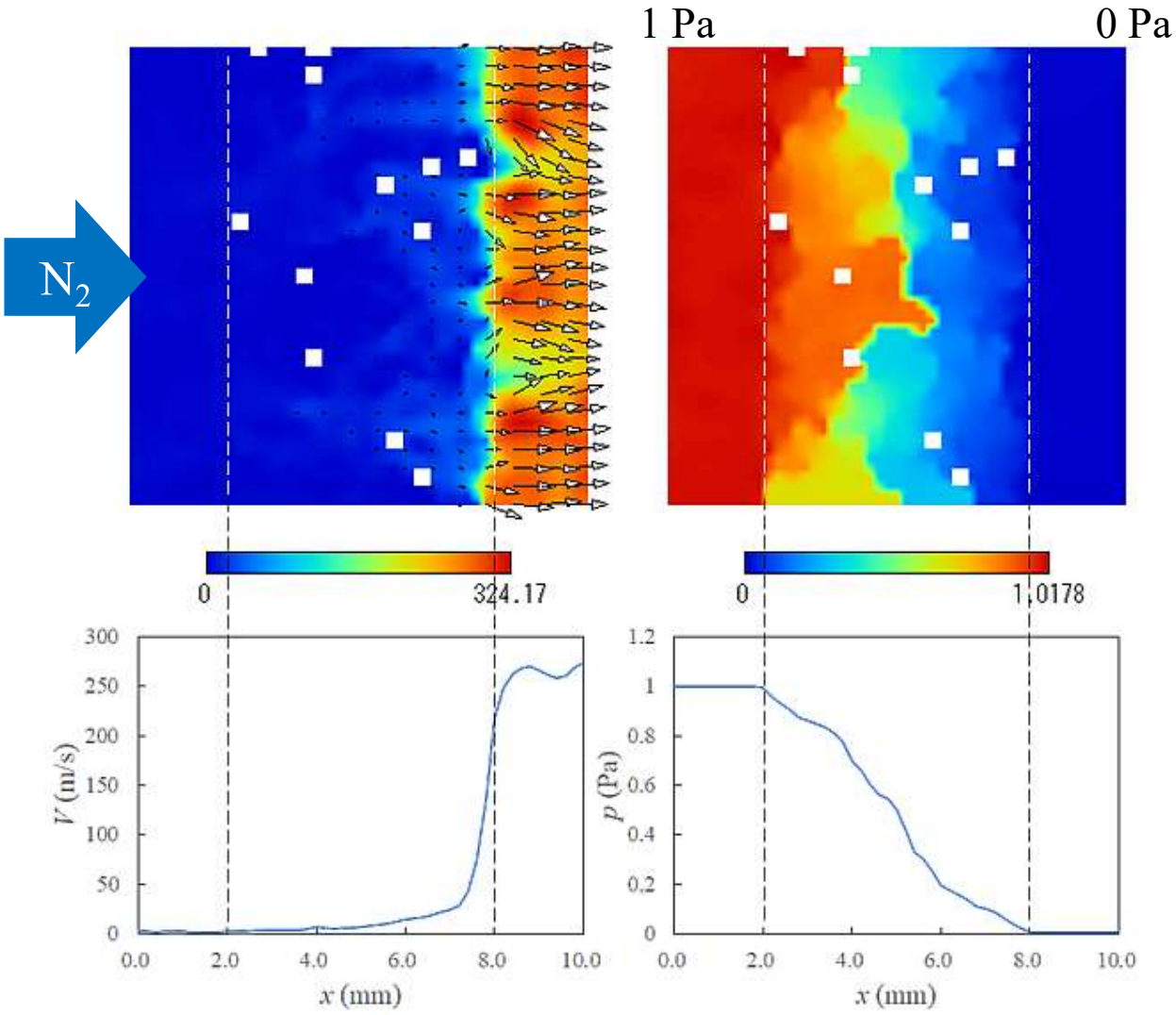
Background

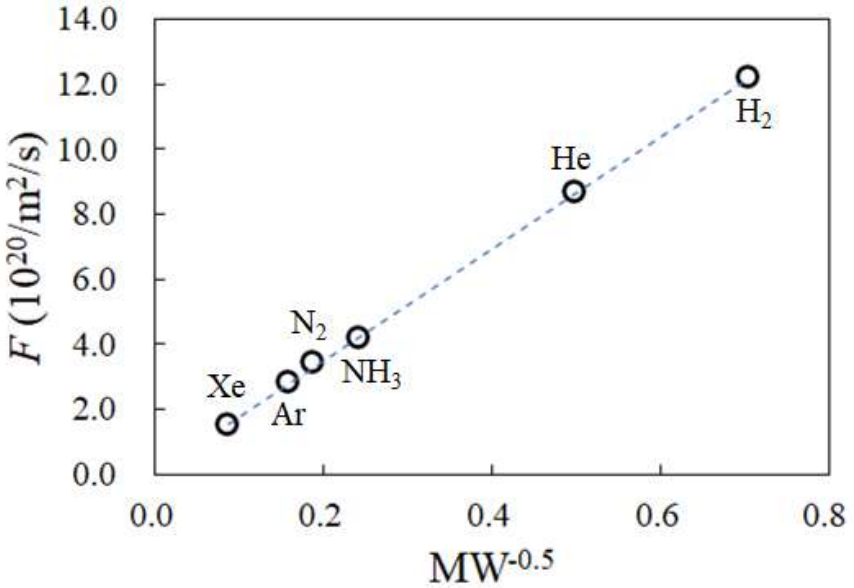
- Porous media in vacuum
  - Vacuum break filter
  - Standard conductance element
  - Perforated plate
  - Rough surface …
- Porous media models in DSMC method
  - Random solid cells
  - Packed cylinders (2D) and spheres (3D)
  - CT images



Background (cont'd)

- DSMC example using random solid cells (RSCs)

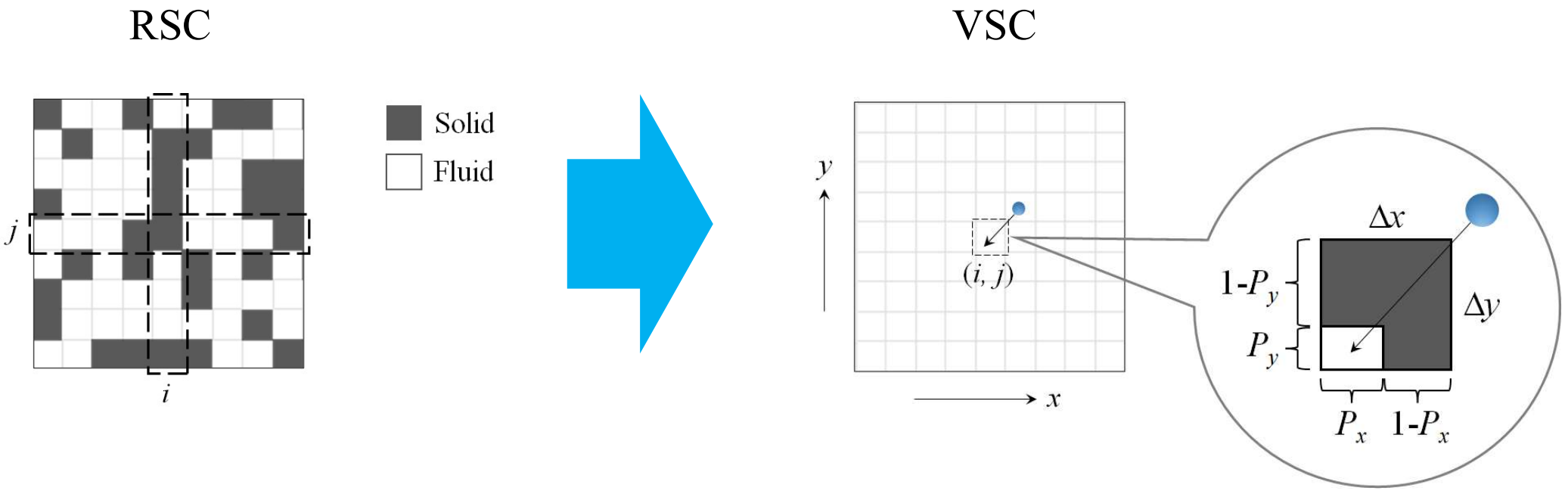




http://www2b.biglobe.ne.jp/~denpoh/Software/DSMC_xls/

Motivation

- Novel porous media model - Virtual Solid Cell (VSC)



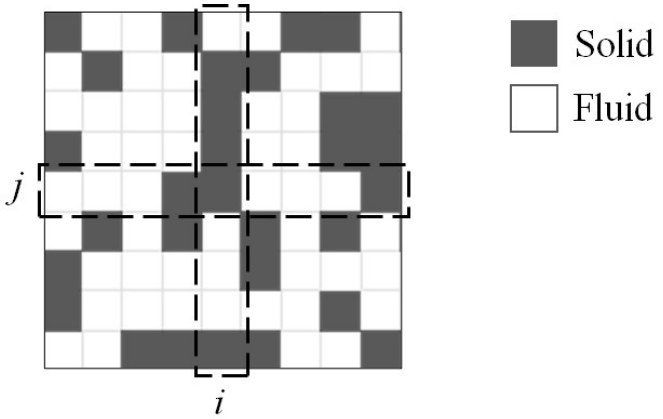
Theory – Random Solid Cell

- Porosity for uniform mesh

$$\varepsilon = \frac{N_\mathrm{f} V_\mathrm{f}}{N_\mathrm{p} V_\mathrm{p}}$$

N: Number of cells, V: Cell volume

f: Fluid, p: Porous media



- In RSC model, $V_\mathrm{f} = V_\mathrm{p}$

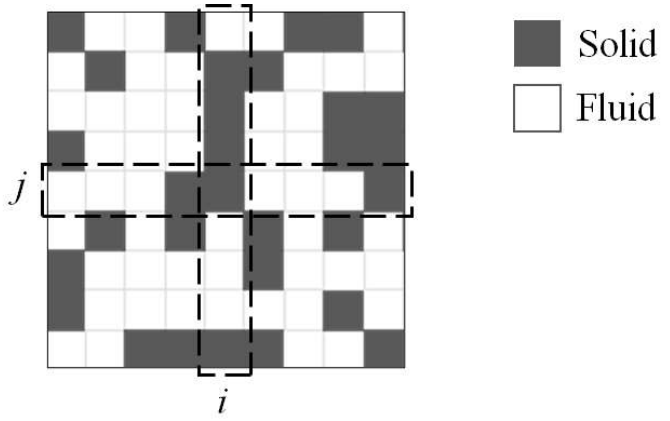
$$\varepsilon_{RSC} = \frac{N_\mathrm{f}}{N_\mathrm{p}}$$

Ratio of # of fluid cells to total # of cells inside porous media

Theory – Virtual Solid Cell

- Porosity for uniform mesh

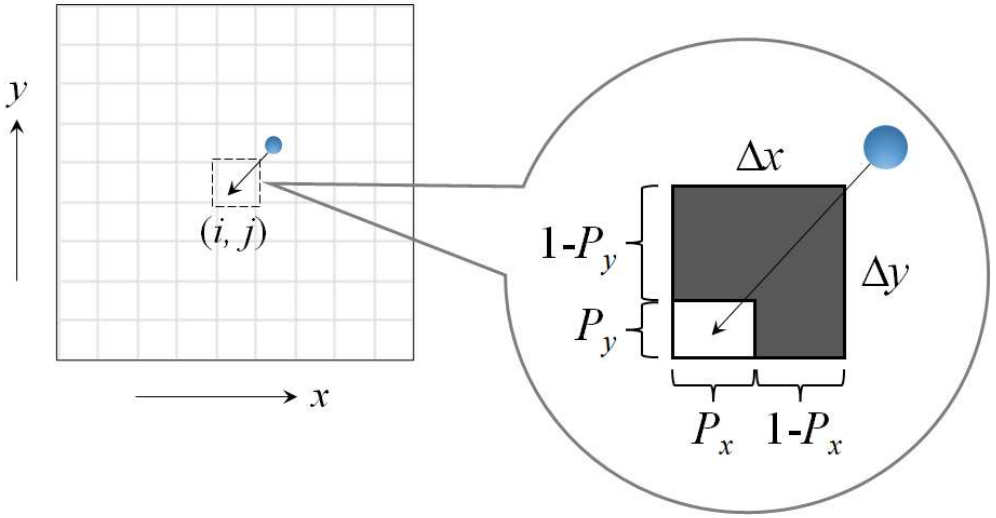
$$\varepsilon = \frac{N_\mathrm{f} V_\mathrm{f}}{N_\mathrm{p} V_\mathrm{p}}$$



- In VSC model, $N_\mathrm{f} = N_\mathrm{p}$

$$\varepsilon_\mathrm{VSC} = \frac{V_\mathrm{f}}{V_\mathrm{p}}$$

Volume fraction of fluid in a cell



- Inter-cell transfer probabilities

$$P_x = \frac{N_{\mathrm{f},i}}{N_{\mathrm{p},i}} = \varepsilon_{\mathrm{RSC},i} \qquad P_y = \frac{N_{\mathrm{f},j}}{N_{\mathrm{p},j}} = \varepsilon_{\mathrm{RSC},j}$$

Theory – Virtual Solid Cell (cont'd)

- Fluid volume in a cell

$$V_{\mathrm{f}} = (P_x \Delta x)(P_y \Delta y)$$

$$= \varepsilon_{\mathrm{RSC},i}\varepsilon_{\mathrm{RSC},j} V_{\mathrm{p}}$$

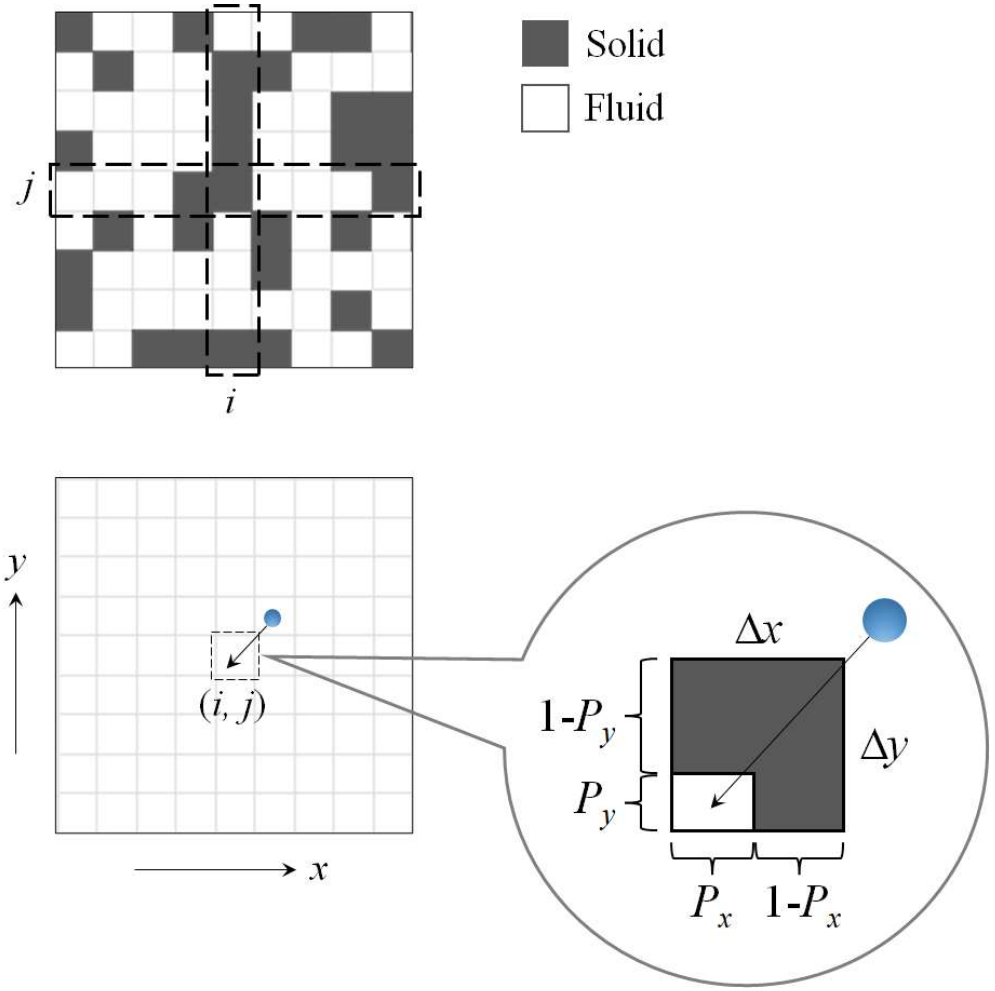
- Therefore,

$$\varepsilon_{\mathrm{VSC}} = \frac{V_{\mathrm{f}}}{V_{\mathrm{p}}} = \varepsilon_{\mathrm{RSC},i}\varepsilon_{\mathrm{RSC},j}$$

- For uniform porous media

$$\varepsilon_{\mathrm{VSC}} = \varepsilon_{\mathrm{RSC}}^2 \quad \text{for 2D}$$

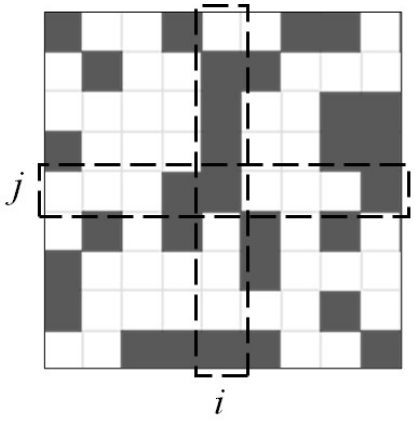
$$(\varepsilon_{\mathrm{RSC}}^3 \quad \text{for 3D})$$



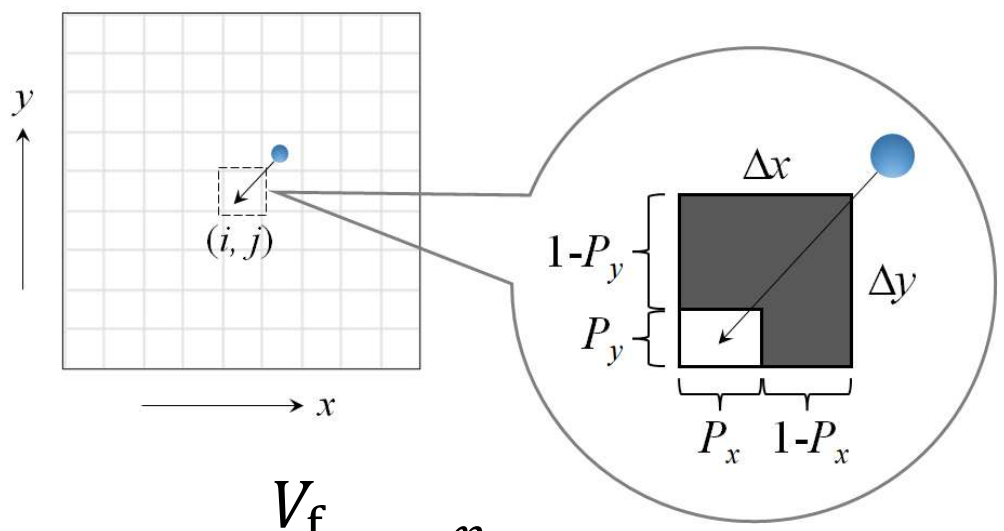
Theory – Brief Summary

- RSC can be replaced with stochastic procedure in VSC

RSC



VSC



$$\varepsilon_{\mathrm{RSC}} = \frac{N_{\mathrm{f}}}{N_{\mathrm{p}}}$$

Ratio of # of fluid cells to total # of cells inside porous media

$$\varepsilon_{\mathrm{VSC}} = \frac{V_{\mathrm{f}}}{V_{\mathrm{p}}} = \varepsilon_{\mathrm{RSC}}^{n}$$

$n = 2$ for 2D

3 for 3D

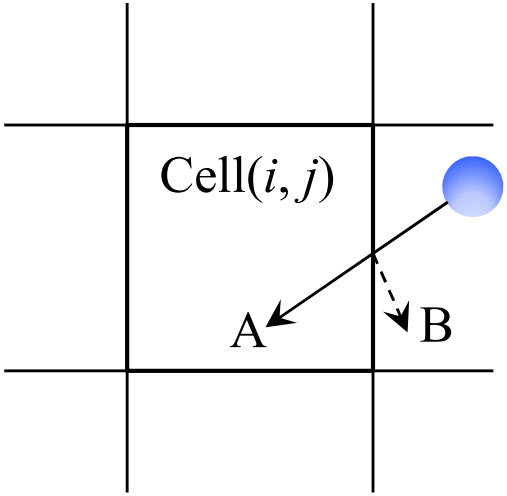
Volume fraction of fluid in a cell

Stochastic Procedure in VSC

- When a gas molecule reaches a cell(i, j) boundary
  - Call a uniform random number U [0,1]

A) If $U \leq \varepsilon_{\mathrm{VSC}}(i, j)$
  - the gas molecule can go inside cell(i, j)

B) Else
  - reflection / sticking / reaction at the boundary



Limitation

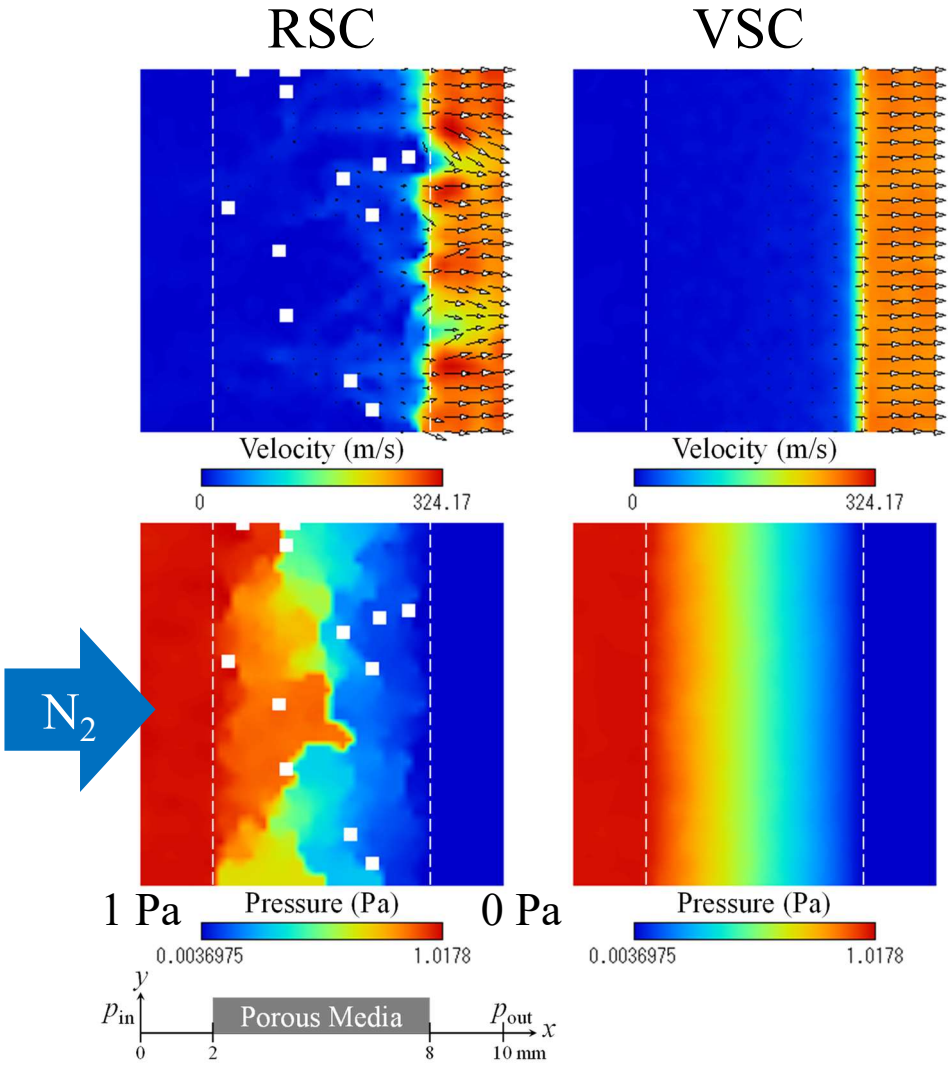
- VSC should be used under following condition,

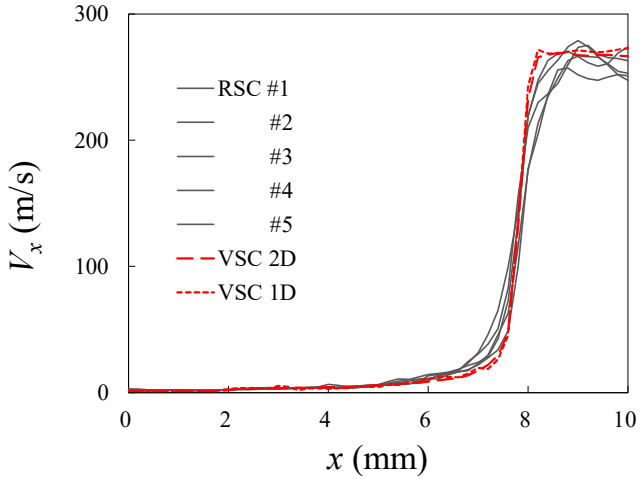
$$\lambda \geq \max(\Delta x, \Delta y, \Delta z),$$

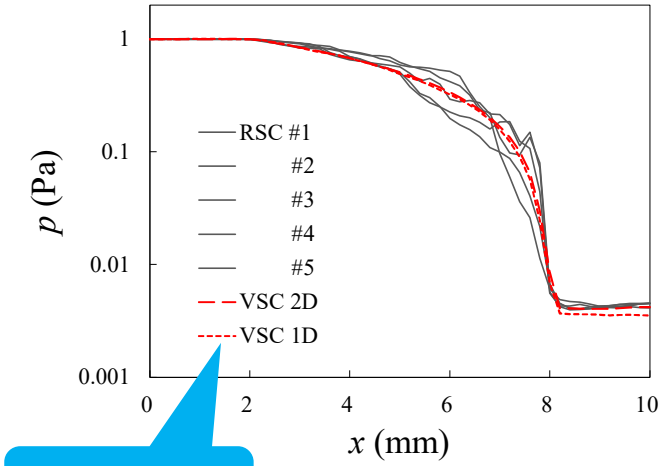
which is the same for DSMC

Application Example #1

- N_2 flow passing through a porous media wall ($\varepsilon_{RSC} = 0.673$)





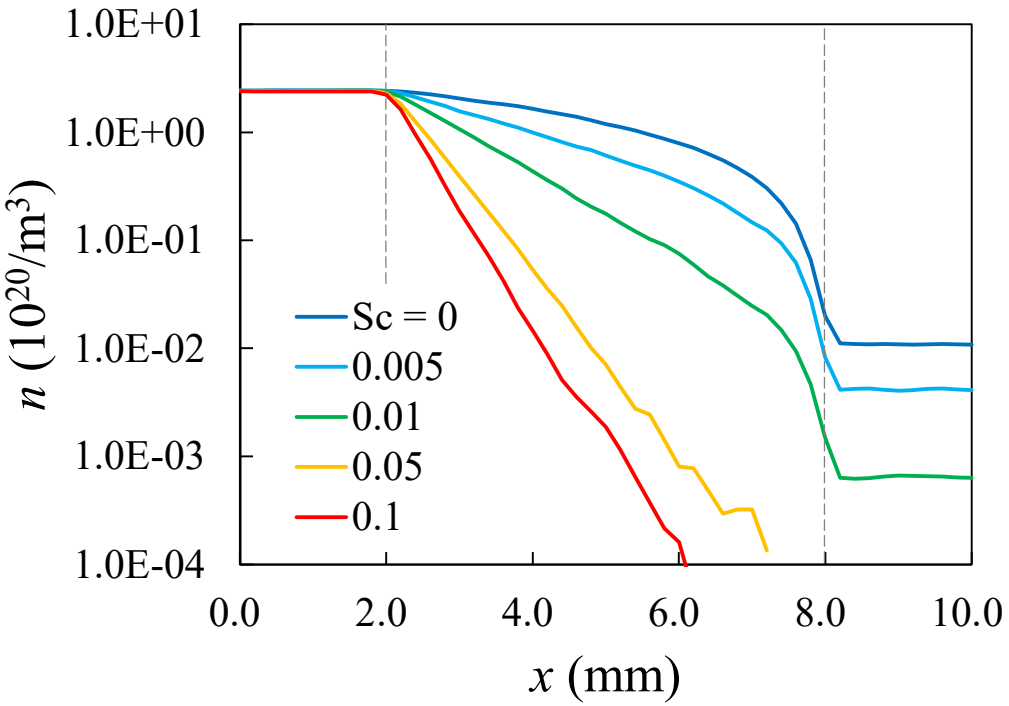


x20 faster

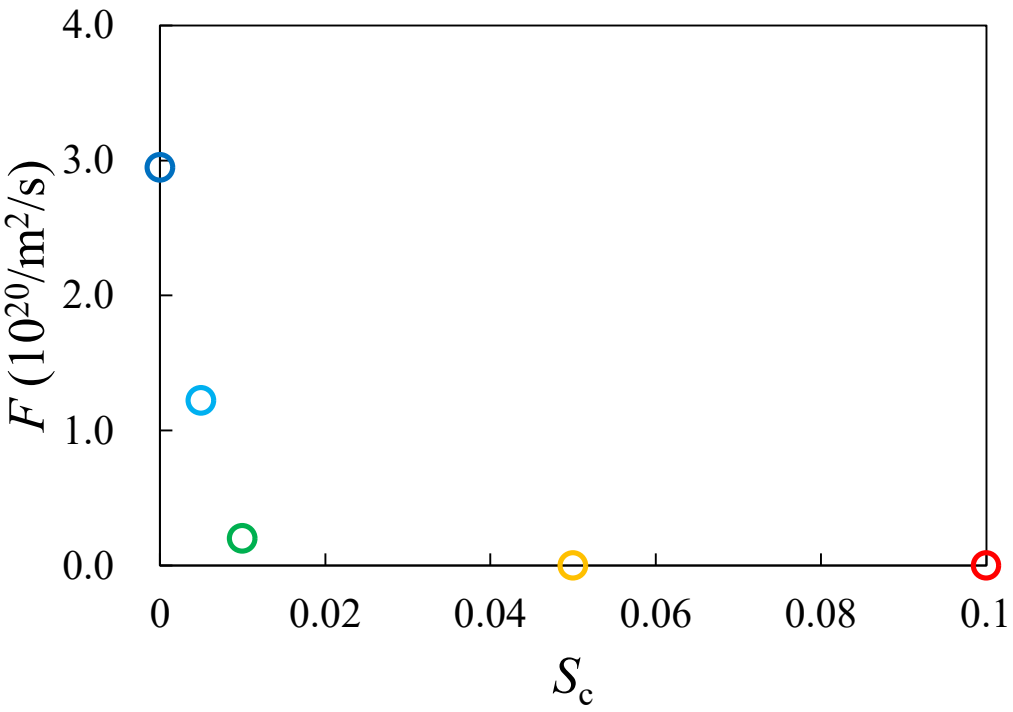
Application Example #1 (cont'd)

- Effects of sticking coefficient (S_c) of porous media wall
  - 1D simulation using VSC model

N_2 number density profile

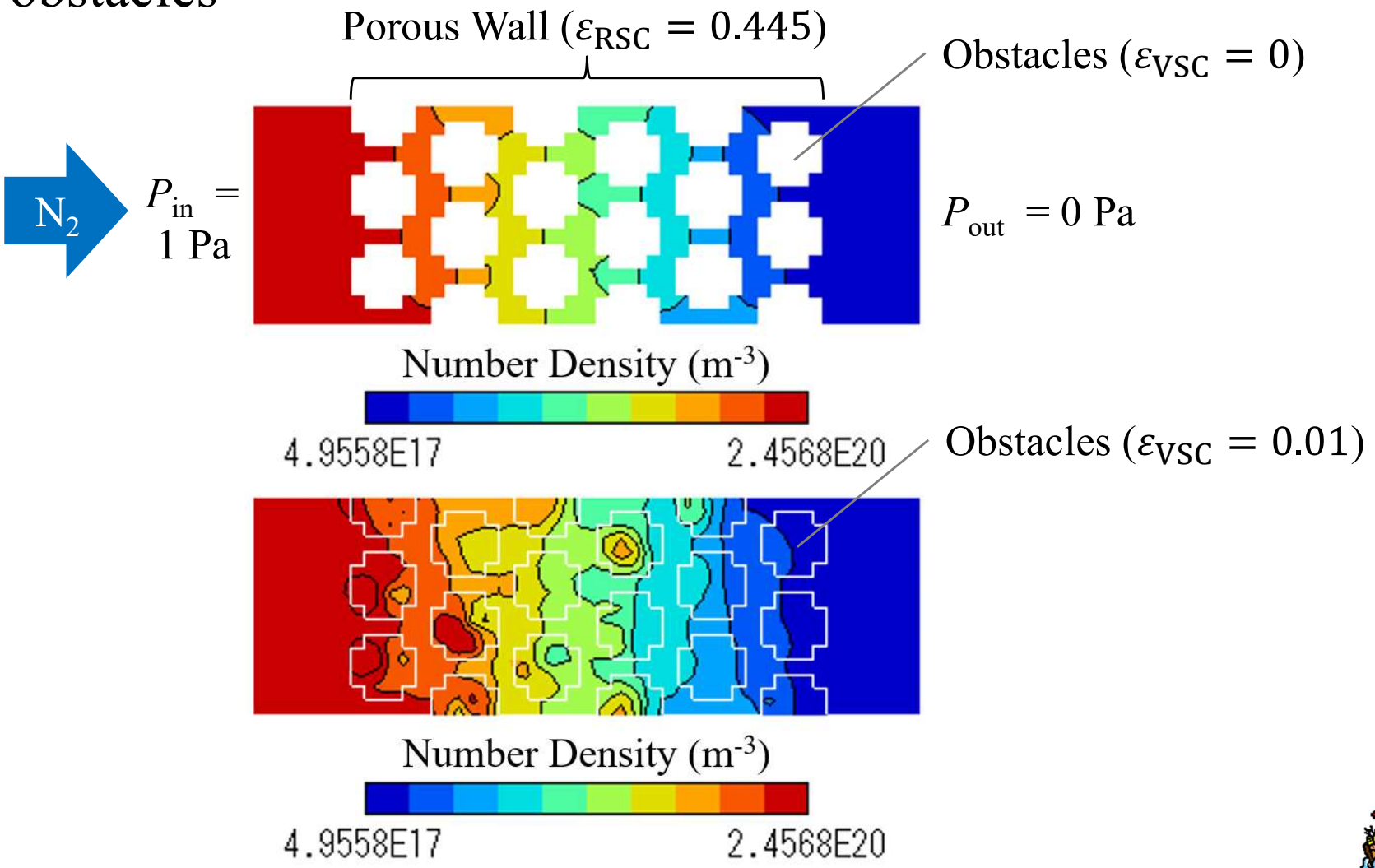


Flux at outlet (x = 10 mm)



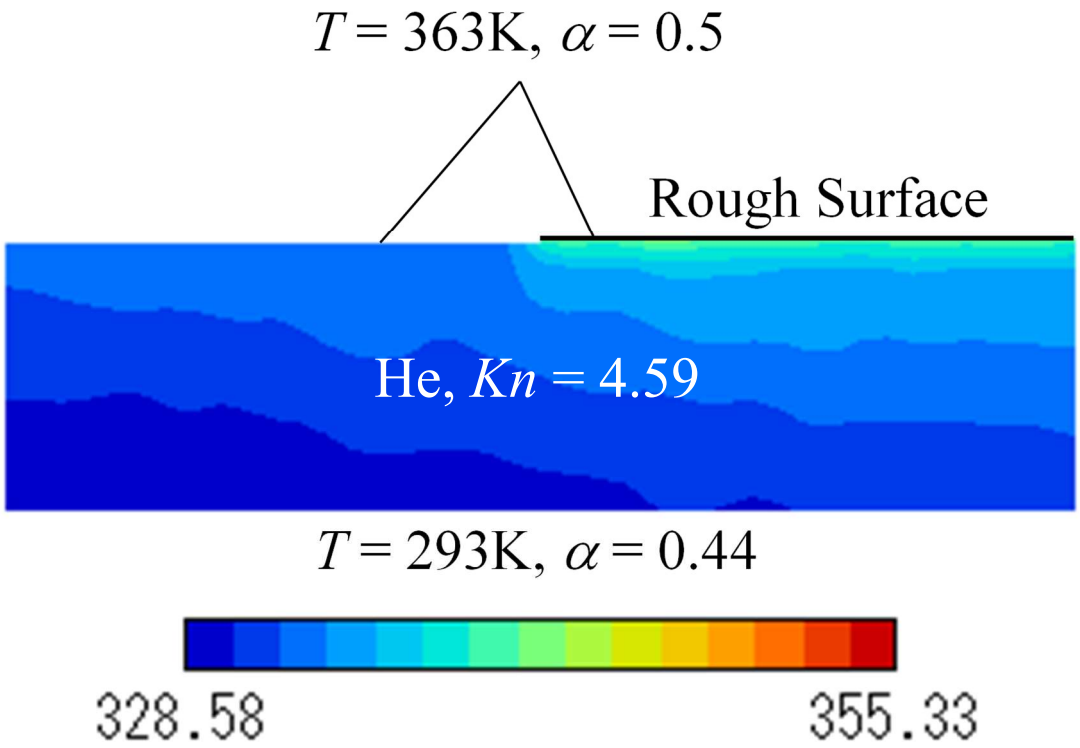
Application Example #2

- N_2 flow passing through a porous media wall formed with multiple porous obstacles



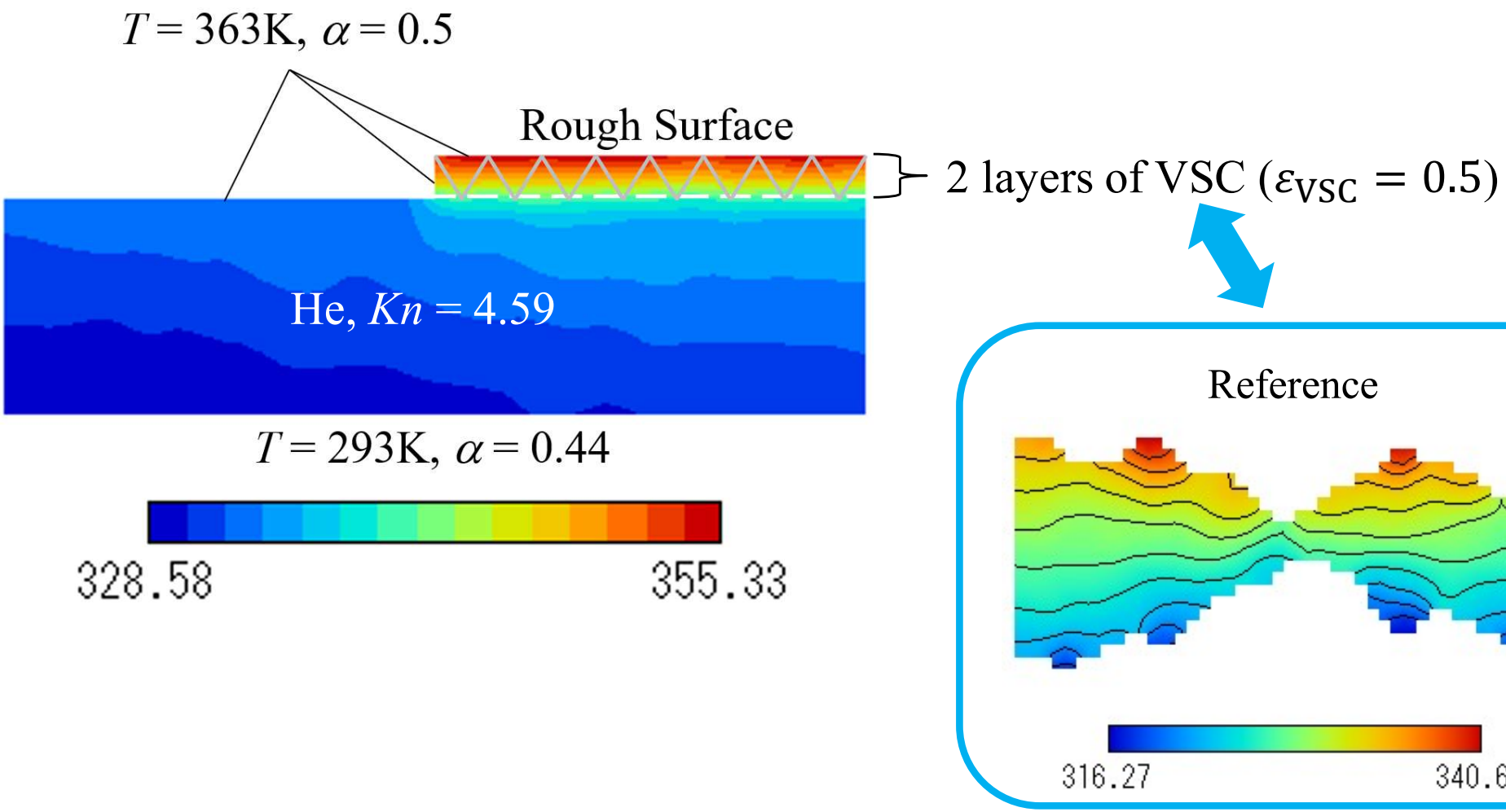
Application Example #3

- He gas temperature between parallel plates



Application Example #3 (cont'd)

- Actual modeling of surface roughness with VSC



Conclusion

- Virtual Solid Cell (VSC) can be used to model
  - porous media
    - 1D
    - porous media with multiple/mixed porosities
  - surface roughness
  - etc...

  in DSMC

- VSC makes DSMC more practical

Thank You

- Ref: K. Denpoh, Vac. Surf. Sci. **66**, 490 (2023).