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Solid Diffusion Modelling

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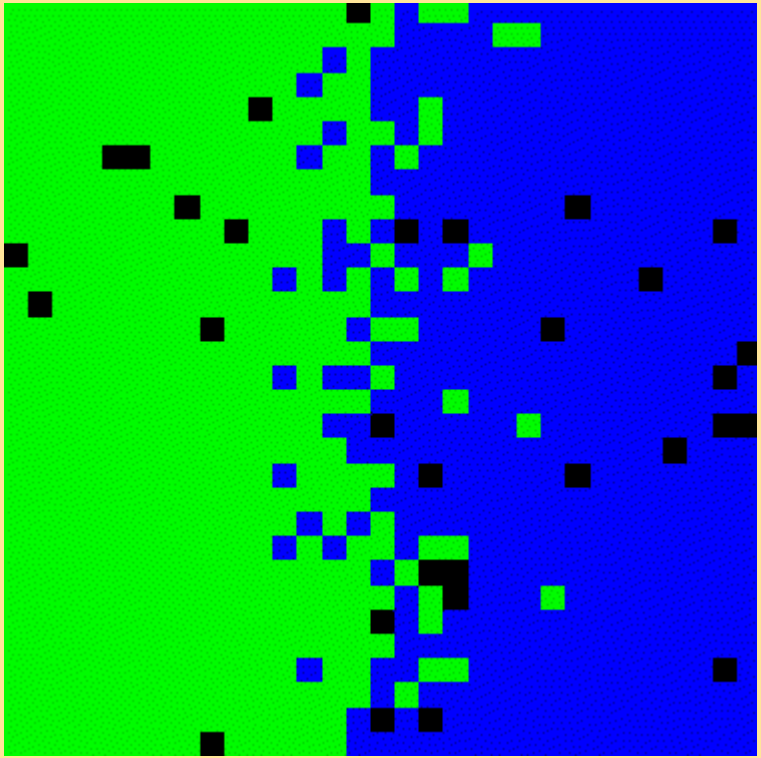
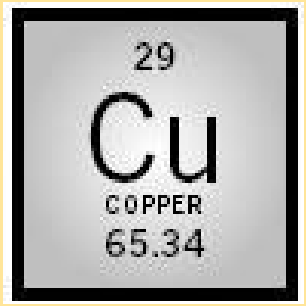
Environmental Modelling - 2014

What is it?

It describes how diffusion occurs between two adjacent solids.



How does it work?



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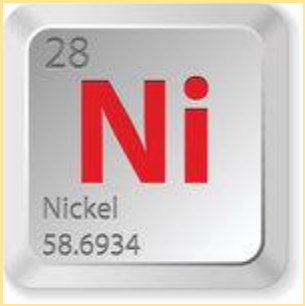


Mechanism:

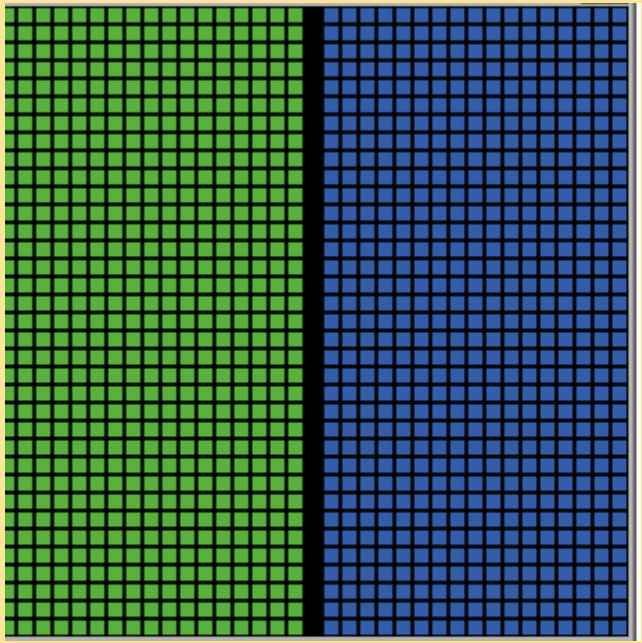
diffusion is caused by missing atoms in the metal crystal.

Model Components:

vacancy

solid 1

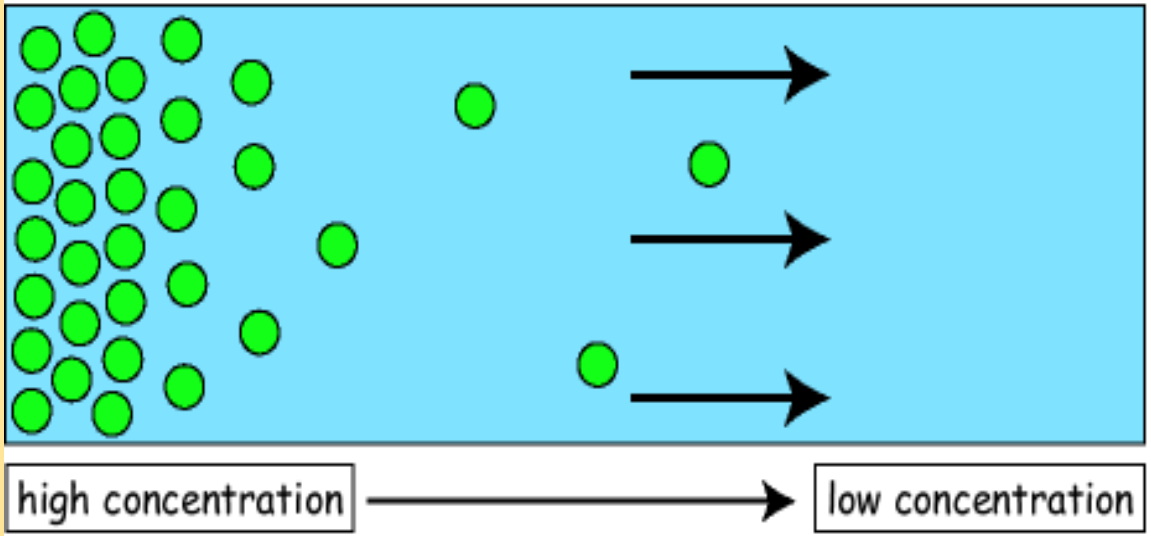
solid 2



Model Assumptions:

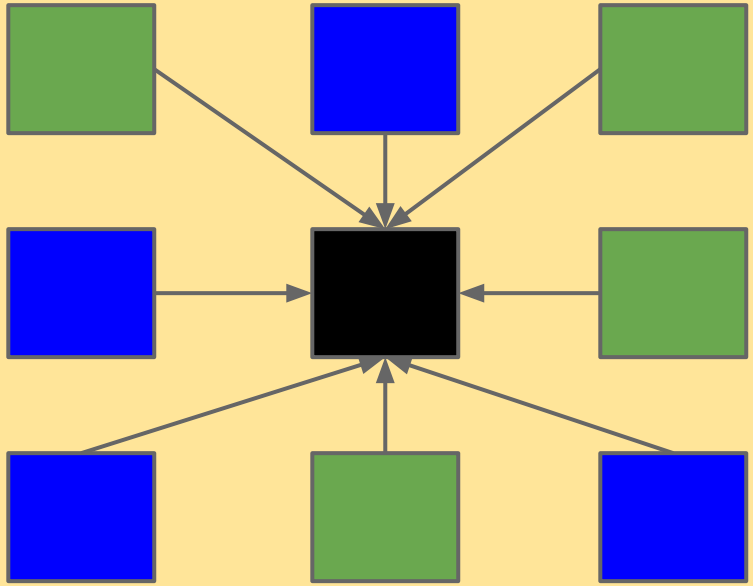
1. similar atomic size,
2. similar crystal structure,
3. similar electronegativity,
4. materials have no vacancies at the beginning,
5. equal heat distribution through the metals.
6. #of vacancies, solid_1, and solid_2 are ALWAYS constant.

Diffusion

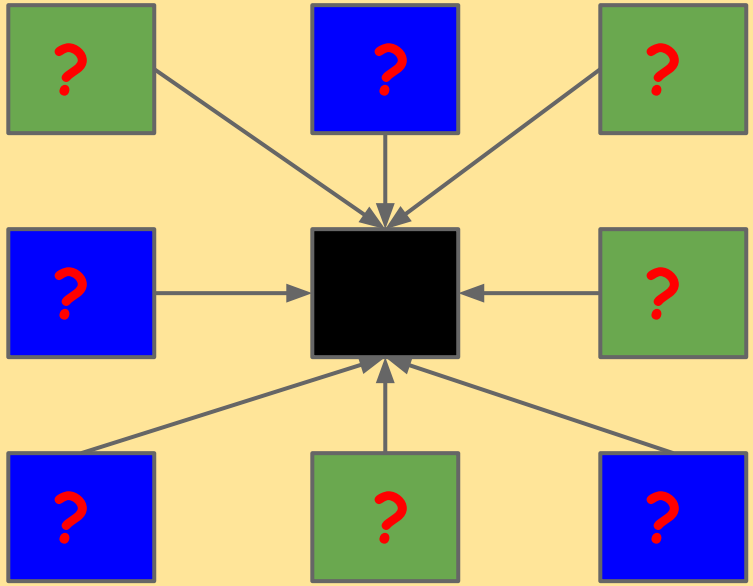


High concentration: atom

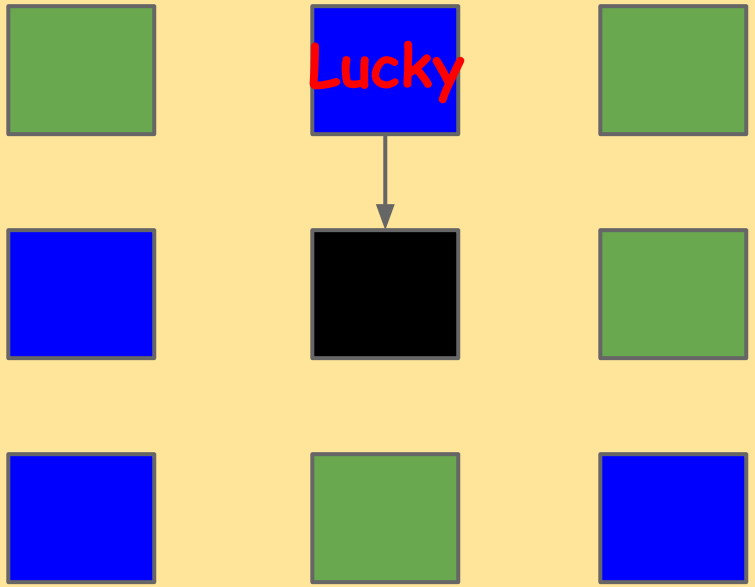
Low concentration: vacancy

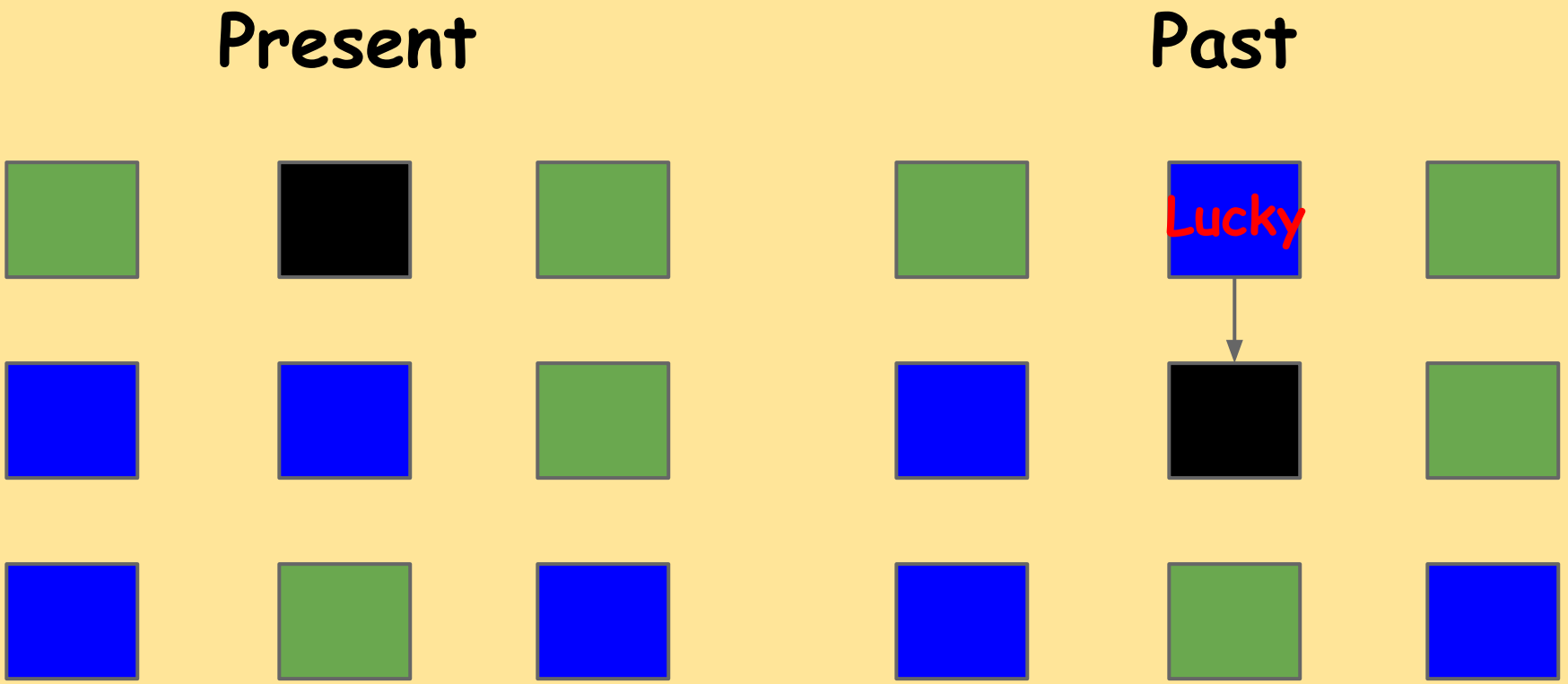


Who will move ?!



Randomly !




Present
Past
Lucky

Model parameters:

of vacancies (1 col., 2 col.s),

neighborhood strategy (moore, von neumann)

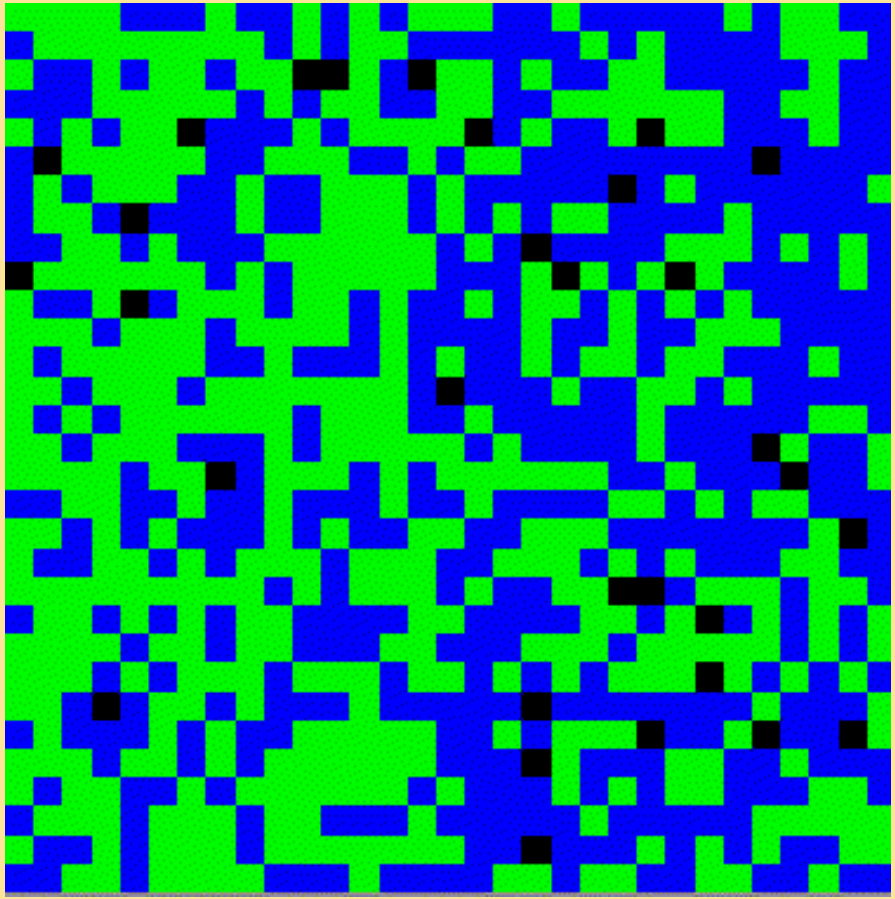

DEMO

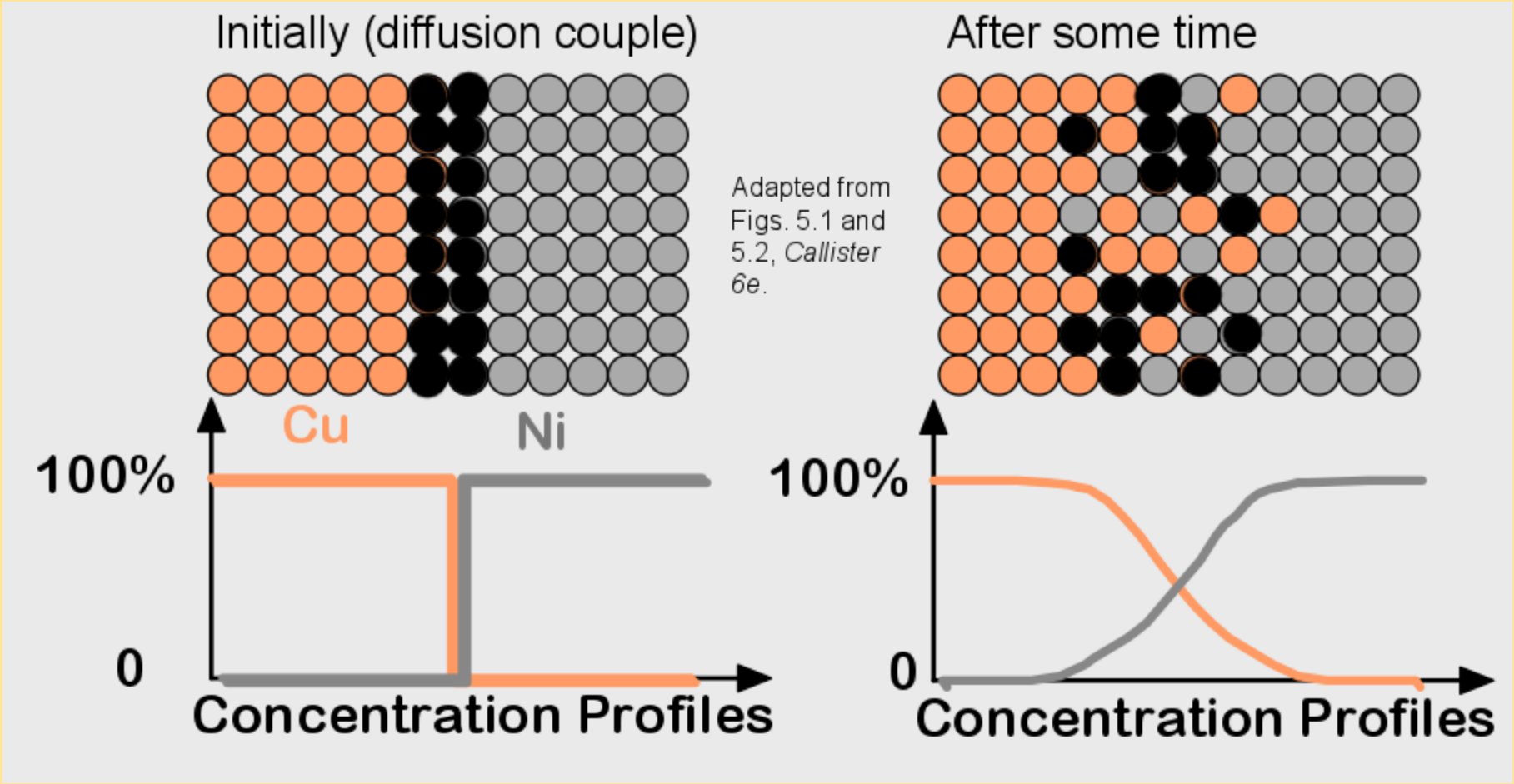
in neighborhood:

$$\text{concentration} = \frac{\#\text{of cells of the same type}}{\#\text{of cells of the neighbourhood}}$$

in grid:

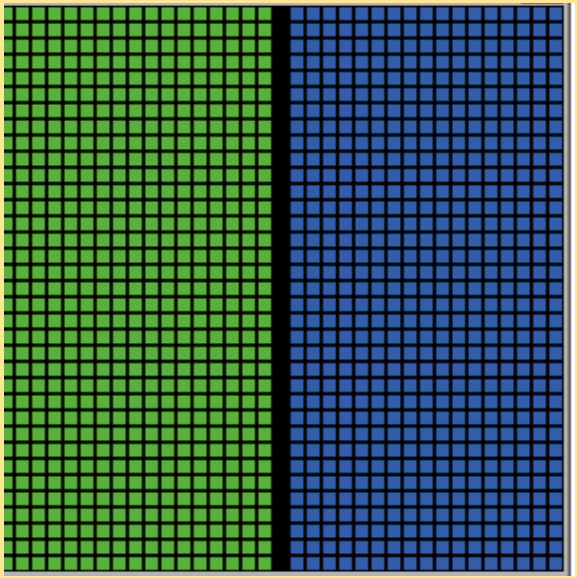
$$\text{concentration index} = \frac{\text{concentration}}{\#\text{of cells of the grid}}$$



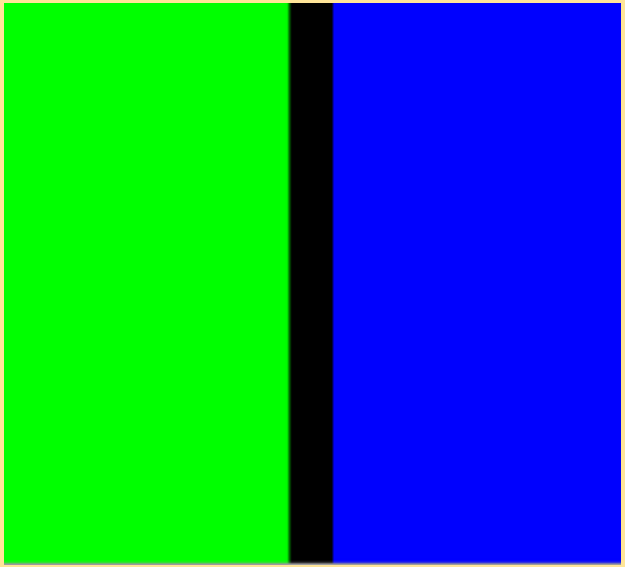

Initially (diffusion couple)
After some time
Adapted from Figs. 5.1 and 5.2, *Callister 6e*.
Cu
Ni
100%
0
Concentration Profiles
100%
0
Concentration Profiles

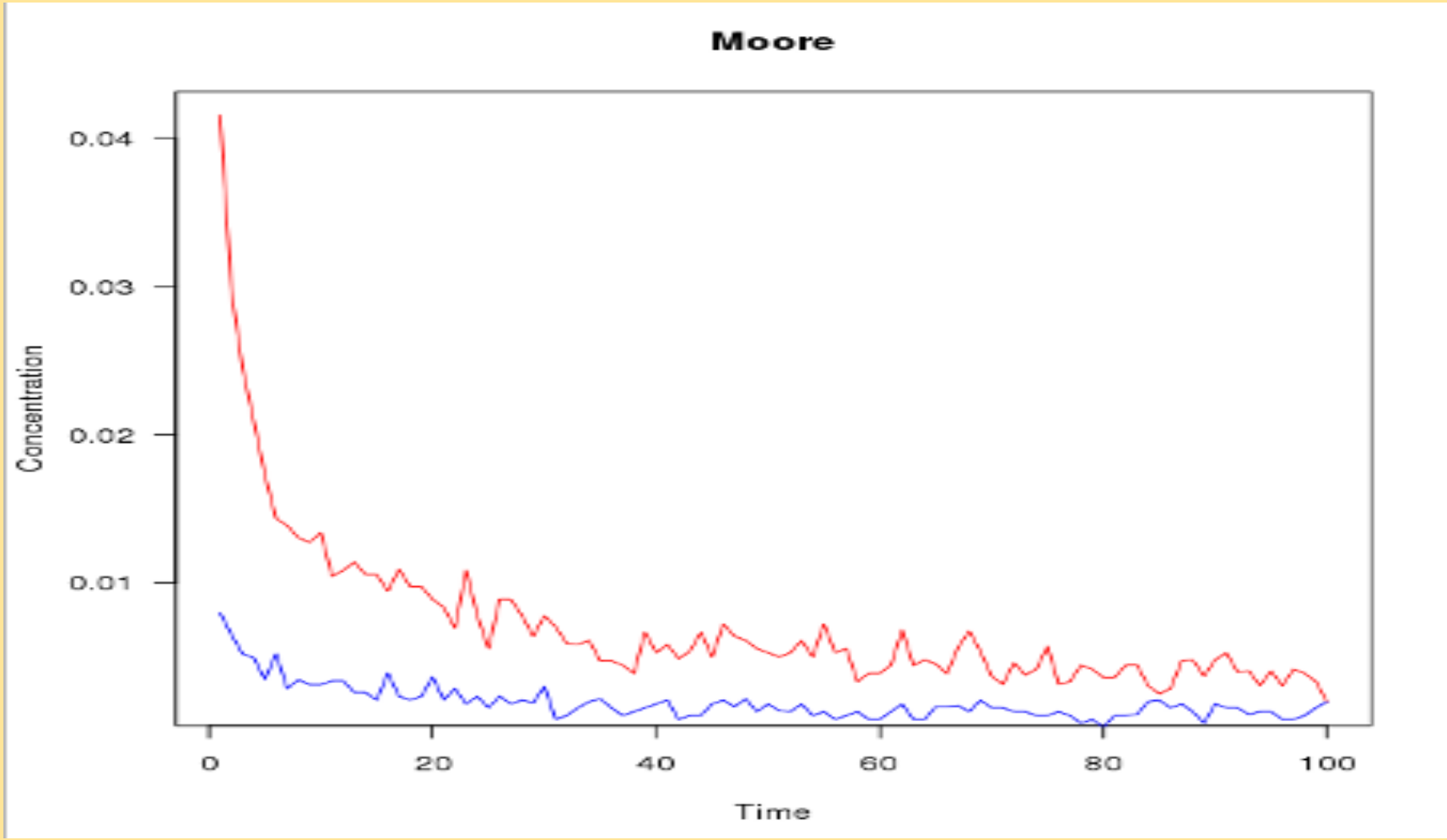
Analysis:

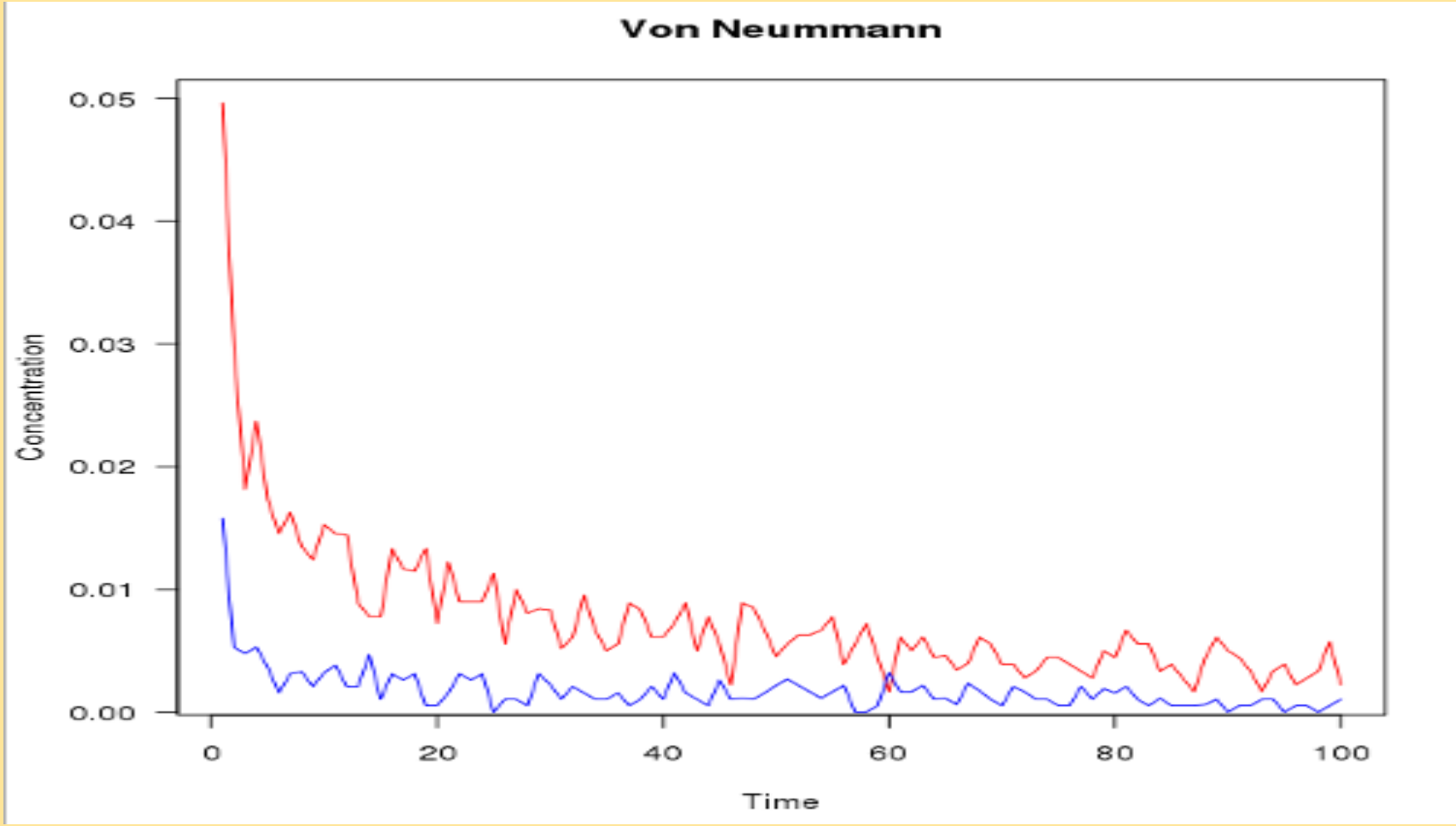
1 col. of vacancies
- moore
- vorneurmann



2 col. of vacancies
- moore
- vorneurmann



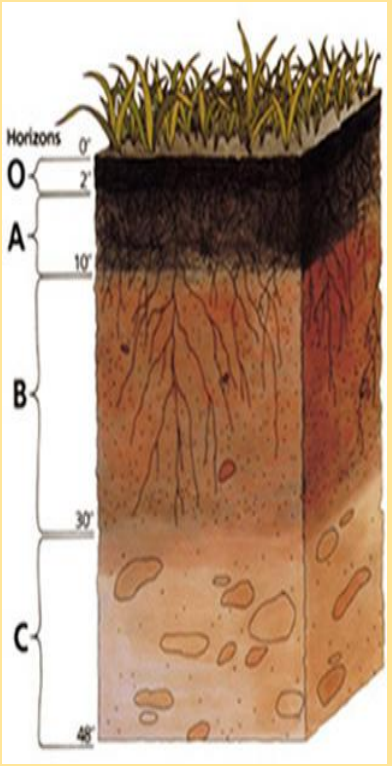

Moore
0.04
0.03
0.02
0.01
Concentration
0
20
40
60
80
100
Time


Von Neummann
Concentration
0.05
0.04
0.03
0.02
0.01
0.00
0
20
40
60
80
100
Time

Why important ?

Applied in many fields:

PHYSICS



Future enhancements:

- consider solid temperatures and atomic size

- try different diffusion mechanisms.

TerraMe features:

cellular space,

observer,

timer,

legend

References:

Google scholar,
NetGeo


THANKS!