Modeling Impurity Migration in Multilayer Systems Using Parallelization

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- We present migration of chemical impurities in a multilayer system
- We try to improve execution times when the simulation is repeated a large number of times

Mathematical model

- Fick's Law of Diffusion:

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- Initial concentration :

$$c(x,0) = c_0(x)$$

Boundary conditions:

$$\left.\frac{\partial c}{\partial x}\right|_{x=0} = 0$$

Interlayer condition (partition coefficient):

$$\frac{c_A(x = L_A)}{c_B(x = L_A)} = K_{AB}$$

Mathematical model

- Finite Differences equation (Crank-Nicolson):

$$\frac{c_i^{n+1} - c_i^n}{\delta t} = D \left[\frac{c_{i-1}^{n+1} - 2c_i^{n+1} + c_{i+1}^{n+1}}{2\delta x^2} + \frac{c_{i-1}^{n} - 2c_i^{n} + c_i^{n}}{2\delta x^2} \right]$$

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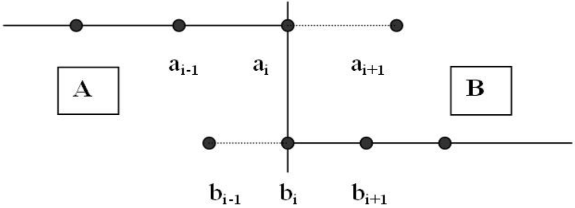
- Fictitious point method



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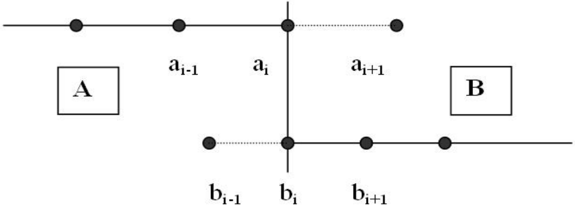
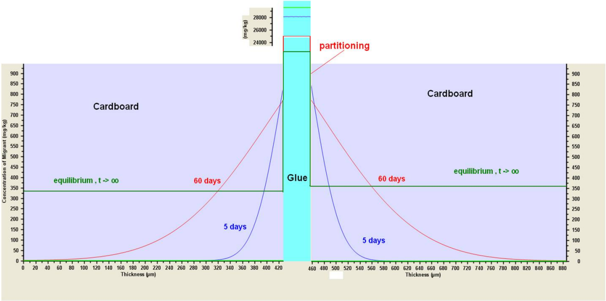


- We end up solving a system of equations

$$\mathbf{Ac^{n+1}} = \mathbf{Bc^n}$$

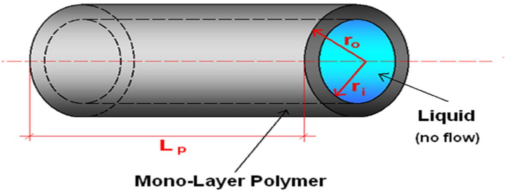
Mathematical model

Figure 1: Planar configuration : cardboard-glue-cardboard.



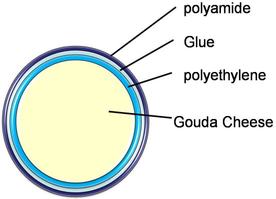
Mathematical model

Figure 2: Cylindrical configuration.



Mathematical model

Figure 3: Spherical configuration.



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- Main program written in C/C++

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- Race conditions must be avoided

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- After the computation is performed, assemble them into a single data file

Results

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- $S_p = \frac{T_s}{T_p} = 2.4$

	With OpenMP(T_p)	**Without OpenMP(T_s)**
Exec. time(s)	5.2	12.5

Discussion

- We presented a model suitable for modeling migration
- The model was applied for a planar configuration can be (and was) extended for other geometries (cylindrical, spherical)
- Parallelization improved the execution times in shared memory systems
- Can be further extended to distributed memory systems (MPI)
- The work was performed within the EU FP7 Project FACET (Flavorings Additives and food Contact materials Exposure Task)

Thank You !