4 Coupled compartments – an analytical solution for diffusion and reaction kinetics

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Four coupled equilibrium reactions with first order rate constants for forward and backward reactions represent a very general scenario for many real problems(see Fig.1).. It can describe deliberate combinations of reversible chemical reactions and diffusion processes [1].

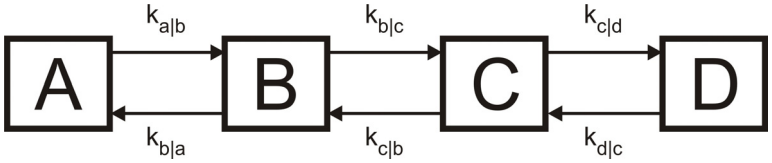

Figure 1: Reversible kinetics between 4 coupled compartments (A, B, C, D) with 8 different

Constants $k_{i;j}$

For each of these processes, a set of differential equations (DES) can be arranged (see eq.1)

and therefore has to be solved.

$$\begin{aligned} d/dt\,(N_A(t)) &= k_{b,a}*(C_B(t)) - k_{a,b}*(C_A(t)) \\ d/dt\,(N_B(t)) &= k_{a,b}*(C_A(t)) - k_{b,a}*(C_B(t)) - k_{b,c}*(C_B(t)) + k_{c,b}*(C_C(t)) \\ d/dt\,(N_C(t)) &= k_{b,c}*(C_B(t)) - k_{c,b}*(C_C(t)) - k_{c,d}*(C_C(t)) + k_{d,c}*(C_D(t)) \\ d/dt\,(N_D(t)) &= k_{c,d}*(C_C(t)) - k_{d,c}*(C_D(t)) \end{aligned} \quad (1)$$

The basic knowledge of solving such DES has been known for more than 200 years. Various numerical methods have been developed as well and lead to excellent result. However, there are situations where an analytical solution is desirable; e.g. backward fitting of parameters or reduction of computational efforts. But we were not able to find an analytical solution for 4 coupled compartments in the published literature. Only advice as to how to solve this problem in general can be found. If anyone is able to provide us with such information we would be very thankful.

Here we have taken the effort to solve the DES that describes the concentration-time profiles for all compartments based on known starting conditions. We validated the results against numerical methods for each of the 4 compartments.

References

[1] H. Barros, J.M. Abril: *Kinetic box models for the uptake of radionuclides and heavy metals by suspended particular matter*. Journal of environmental Radioactivity (**99)**, 146 - 1578 (2008).