# I – Appendix: The INVERSE method - Determination of diffusion coefficients

In the Figure 1 model of interdiffusion in multi-component system is schematically presented. For given initial concentration profiles , thermodynamic data, and diffusion coefficients using the physical laws and boundary conditions model allows to calculated concentration profiles for every time. Diffusion coefficients, particularly in multi-component systems are not known.

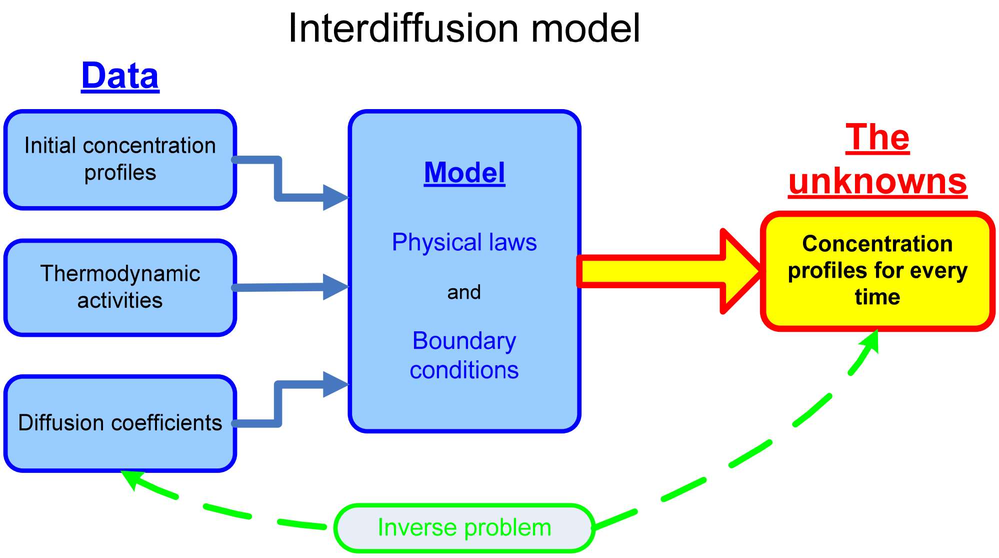


**Figure 1.** Model of interdiffusion in non-ideal systems which allows to calculate concentration profiles for every time.

One of the method, which resolves this problem is so called the Inverse method. It is a semi-empirical approach which requires knowledge of experimental concentration profiles (e.g, from diffusion cauple experiment). The *Inverse* method is based on solution of the inverse problem of interdiffusion, i.e., on finding such coefficients for which calculated profiles match experimental ones with the least error. – Figure 2.

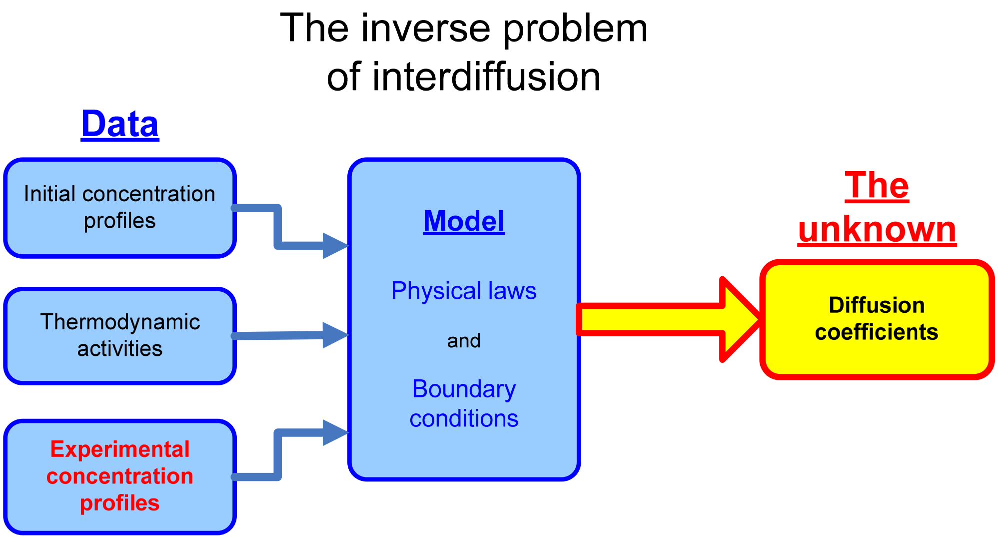


**Figure 2.** The inverse problem of interdiffusion which enables calculation of diffusion coefficients.

A measure of „deviation" of calculated profiles from experimental ones is "distance" between both profiles defined as area between them. This area denotes as $err(D)$ is function, which depends on diffusion coefficients for which the calculations are performed:

$$err(D_1,\ldots,D_r)=\left(\sum_{i=1}^{r} d^{-1}\int_0^d w_i(x)\left(c_i^{eksp}(x)-c_i^{obl}(x,D_1,\ldots,D_r)\right)^2 dx\right)^{1/2} \qquad (1)$$

where $d$ – thickness of the system (diffusion couple), $w_i(x)$ - weight functions (presently equals 1), $c_i^{eksp}(x)$ - experimental concentration profile, $c_i^{obl}(x,D_1,\ldots,D_r)$ - calculated profile using diffusion coefficients $D_1,\ldots,D_r$ as given parameters.

Determination of diffusivities is equivalent to finding parameters $\phi_i^{\cdots}$ (see Appendix H). For example for ternary system we look for 24 parameters (12 for $D_i^o$ and 12 for $E_i$ ). Method of determination of the above parameters is carried out by minimization of the error function (1). Parameters $\phi_i^{\cdots}$, which minimize function (1) after inserting Redlich-Kister polynomials are looked for diffusion coefficients $D_i$ .