SIMULATION OF THE CONCRETE CHLORIDE NT BUILD-492 MIGRATION TEST

Juan Lizarazo-Marriaga

P A Claisse

Javier Gonzalez

Aix-en-Provence, France
May 29-June 1, 2012

SSCS 2012
Numerical Modeling
Strategies for Sustainable Concrete Structures

Contents

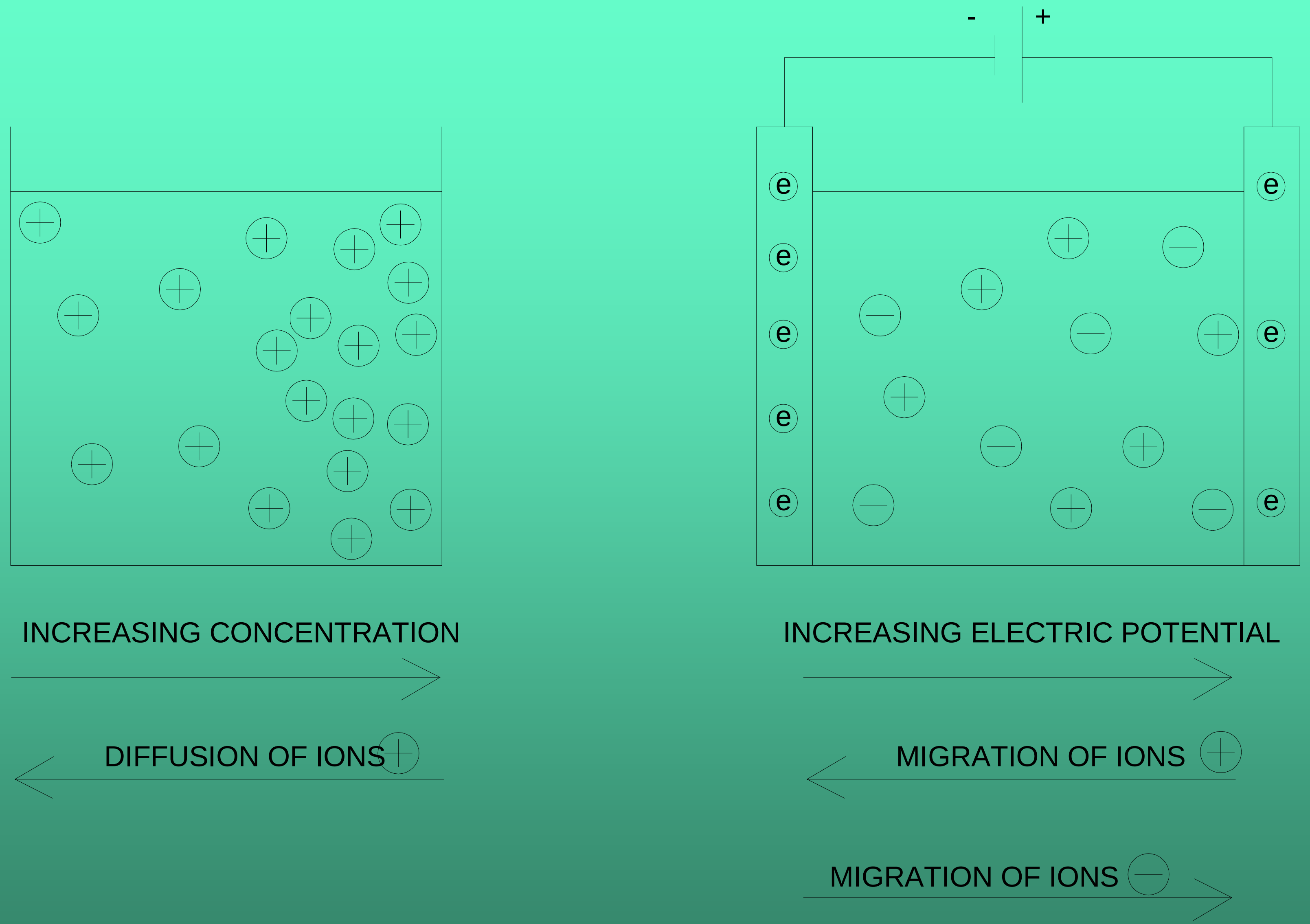
- Nordtest 492 experiment
- Electro-diffusion model
- Simulation results

Justification

- **Corrosion of steel reinforced concrete is caused by chloride ingress**

- **Widespread occurrence and high cost of repair.**

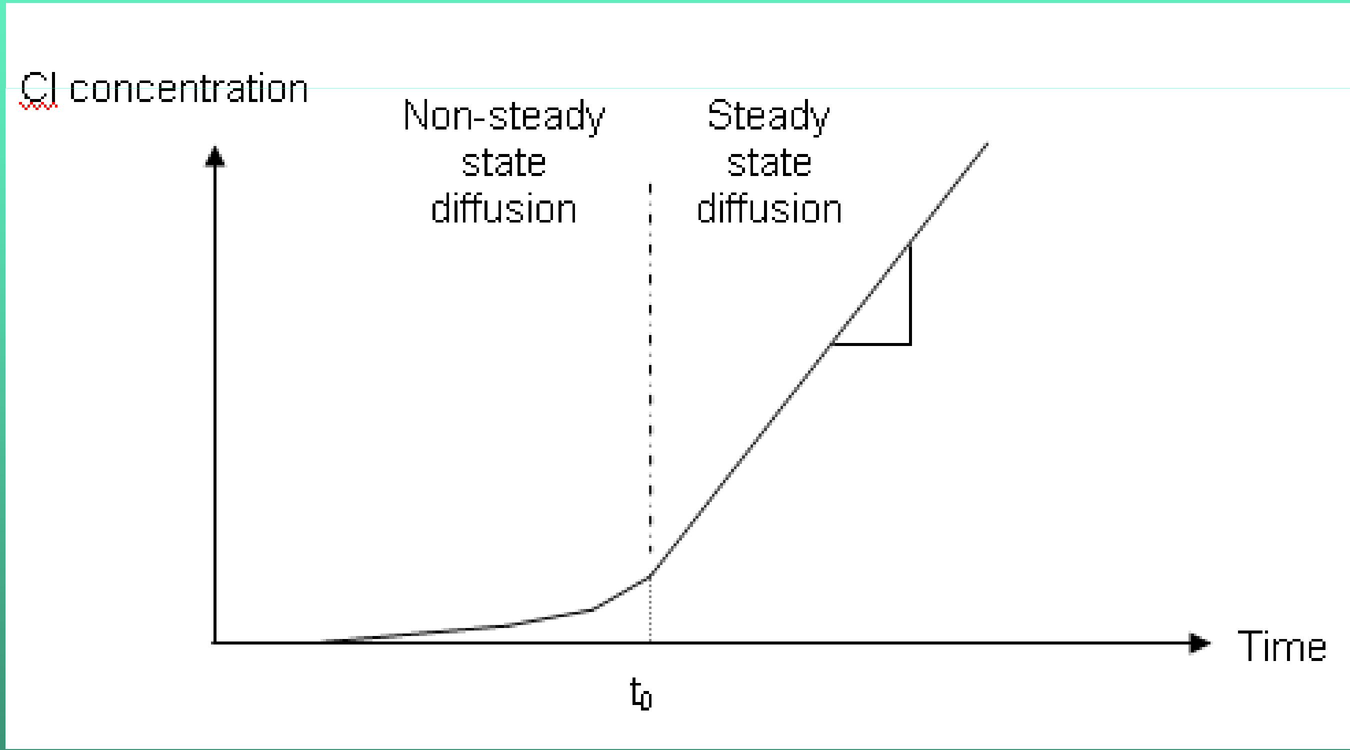
http://www.nace.org/nace/content/library/photogallery/



Schematic representation of the ionic diffusion and migration processes (Bockris and Reddy 1998)

•Fick’s laws

$$J_i = D_i \frac{\partial c_i}{\partial x} \qquad \frac{\partial C_i}{\partial t} = D_i \frac{\partial^2 C_i}{\partial x^2}$$



Ji= flux of species i [mol/m2/s]
Di= diffusion coefficient of i [m2/s]
ci= ionic concentration of i in the pore fluid [mol/m3]
x= distance [m]

•Nernst-Planck equation

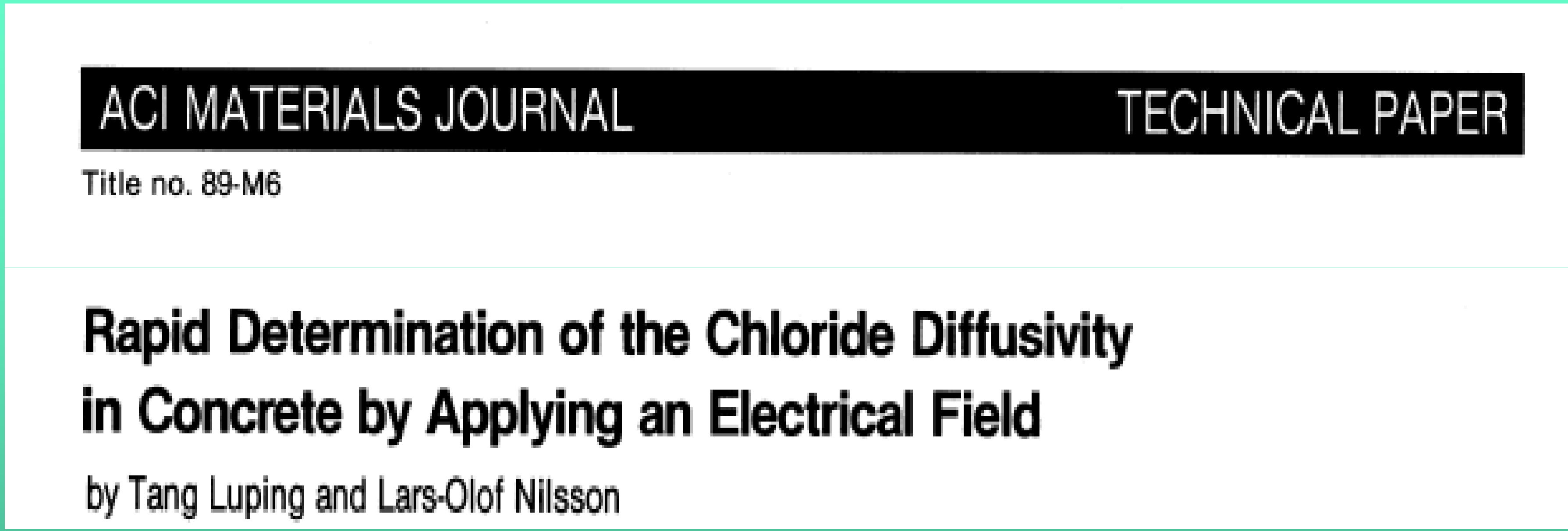
$$J_i = D_i \frac{\partial c_i}{\partial x} + \frac{z_i F}{RT} D_i c_i \frac{\partial E}{\partial x}$$

Diffusion term **Migration term**

$$c(x,t) = \frac{c_s}{2}\left[e^{ax}\,ercf\left(\frac{x+aDt}{2\sqrt{Dt}}\right) + ercf\left(\frac{x-aDt}{2\sqrt{Dt}}\right)\right]$$

$$a = zFE/RT$$

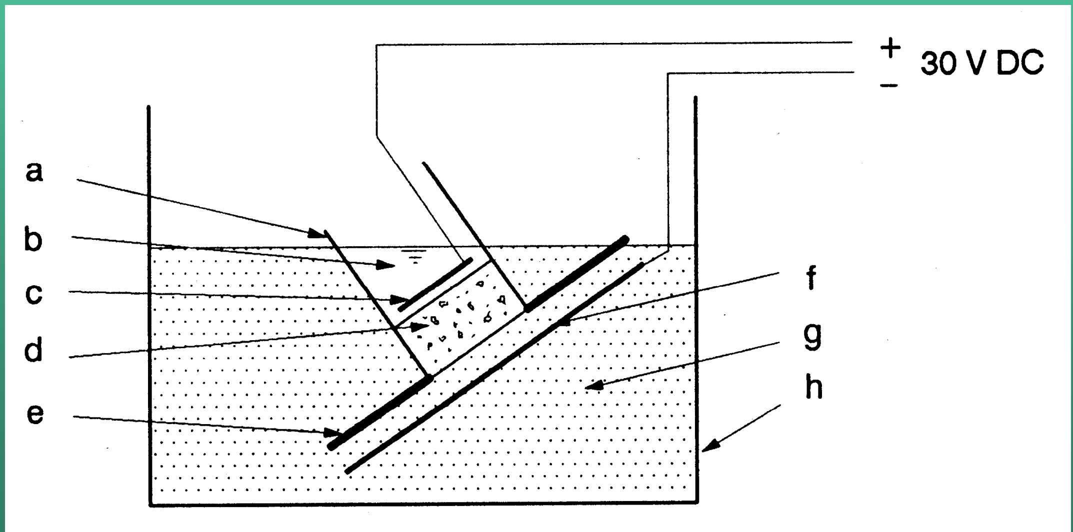
Ji= flux of species i [mol/m2/s]
Di= diffusion coefficient of i [m2/s]
ci= ionic concentration of i in the pore fluid [mol/m3]
x= distance [m]
zi= electrical charge of i,
F= Faraday constant [Coulomb/mol]
R= gas constant [J/mol/ºK]
T= absolute temperature [ºK]
E= electrical potential [V].

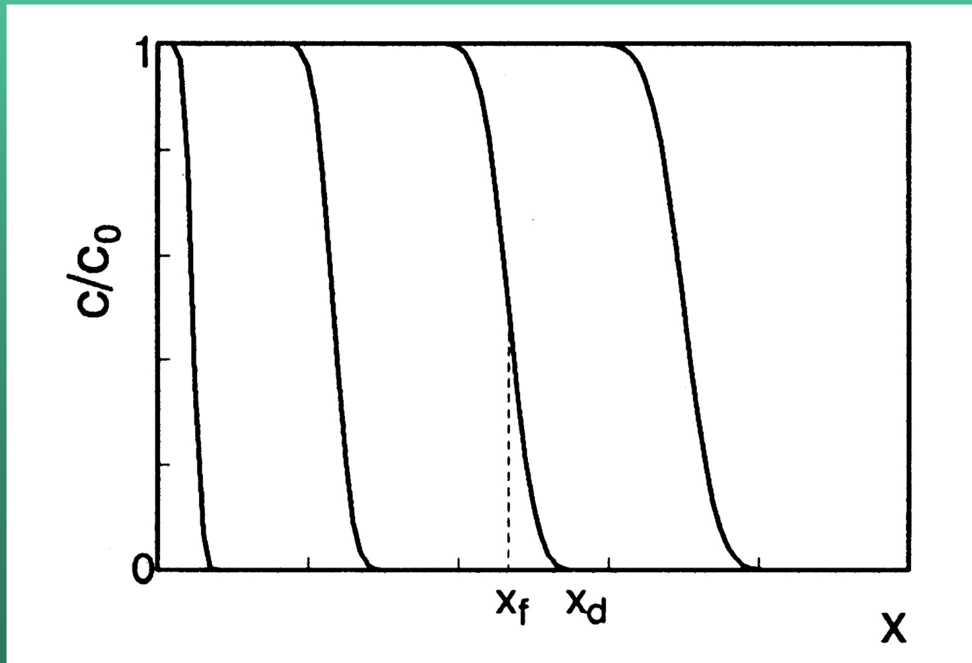

ACI MATERIALS JOURNAL TECHNICAL PAPER

Title no. 89-M6

Rapid Determination of the Chloride Diffusivity in Concrete by Applying an Electrical Field

by Tang Luping and Lars-Olof Nilsson





nordtest method

NT BUILD 492

Approved 1999–11

1(8)

CONCRETE, MORTAR AND CEMENT-BASED REPAIR MATERIALS:
CHLORIDE MIGRATION COEFFICIENT FROM NON-STEADY-STATE MIGRATION EXPERIMENTS

UDC 691.32/691.53/691.54

Key words: Chlorides, concrete, diffusion, mortar, repair materials, migration, test method

1 SCOPE

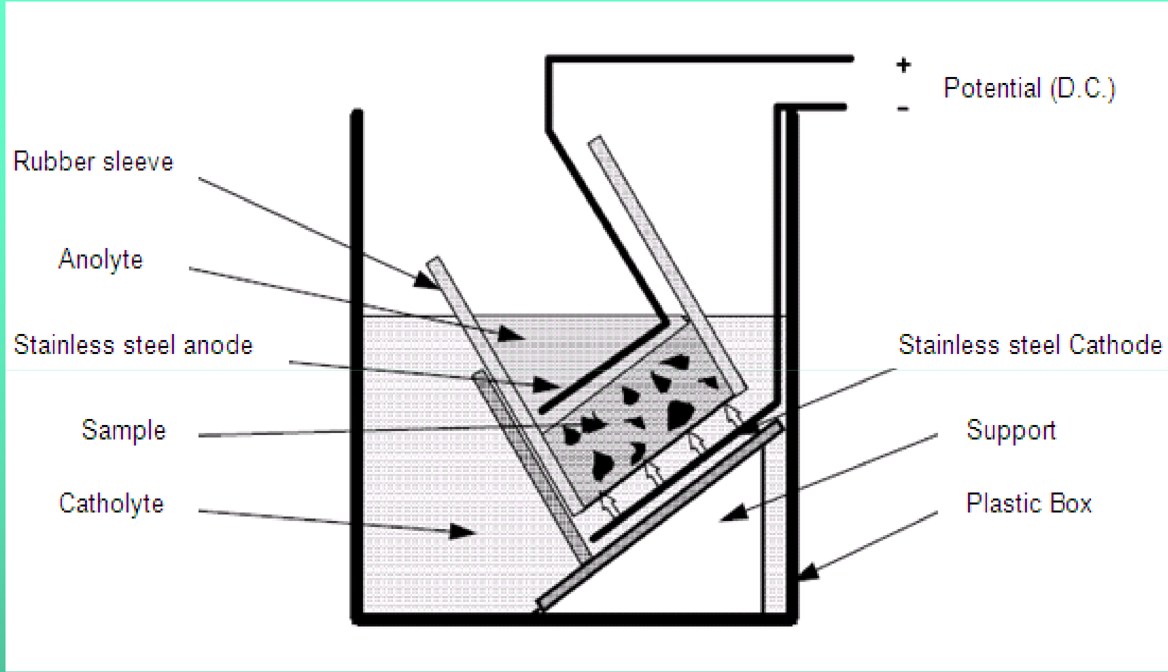
This procedure is for determination of the chloride migration coefficient in concrete, mortar or cement-based repair materials from non-steady-state migration experiments.

5 SAMPLING

The method requires cylindrical specimens with a diameter of 100 mm and a thickness of 50 mm, sliced from cast cylinders or drilled cores with a minimum length of 100 mm. The cylinders and cores should meet the requirements described

SIMULATION OF THE CONCRETE CHLORIDE NT BUILD-492 MIGRATION TEST

J. Lizarazo-Marriaga – P. Claisse – J. Gonzalez



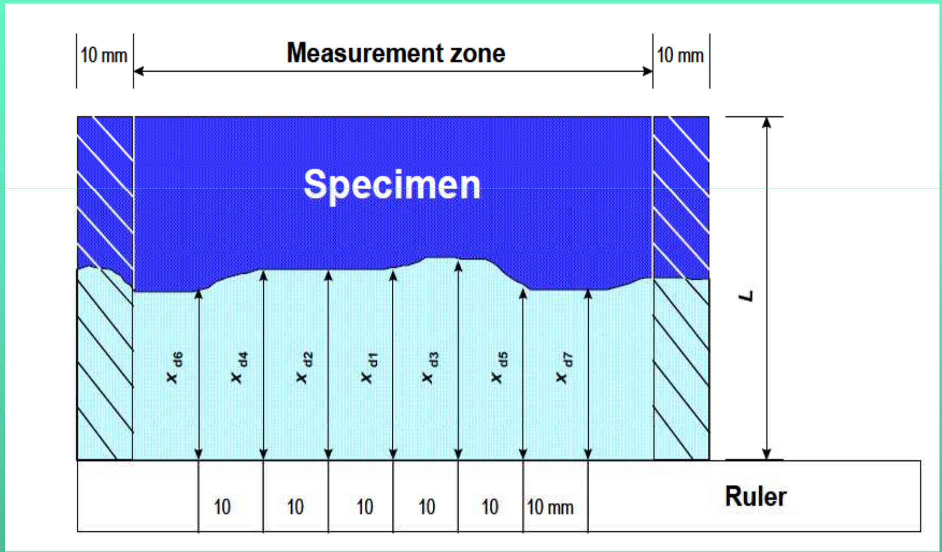
D_{nssm}: non-steady-state migration coefficient, m^2/s;
z: absolute value of ion valence, for chloride, $z = 1$;
F: Faraday constant, $F = 9.648 \times 10^4$ J/(V·mol);
U: absolute value of the applied voltage, V;
R: gas constant, $R = 8.314$ J/(K·mol);
T: average value of the initial and final temperatures in the anolyte solution, K;
L: thickness of the specimen, m;
x_d: average value of the penetration depths, m;
t: test duration, seconds;
erf^{-1}: inverse of error function;
c_d: chloride concentration at which the colour changes, $c_d \approx 0.07$ N for OPC concrete;
c_0: chloride concentration in the catholyte solution, $c_0 \approx 2$ N.

$$D_{nssm} = \frac{RT}{zFE} \cdot \frac{x_d - \alpha\sqrt{x_d}}{t}$$

where:

$$E = \frac{U-2}{L}$$

$$\alpha = 2\sqrt{\frac{RT}{zFE}} \cdot \mathrm{erf}^{-1}\left(1 - \frac{2c_d}{c_0}\right)$$



chloride penetration depths after applying 0.1 N silver nitrate in a chloride contaminated concrete sample

Electro-diffusion model for chlorides in concrete

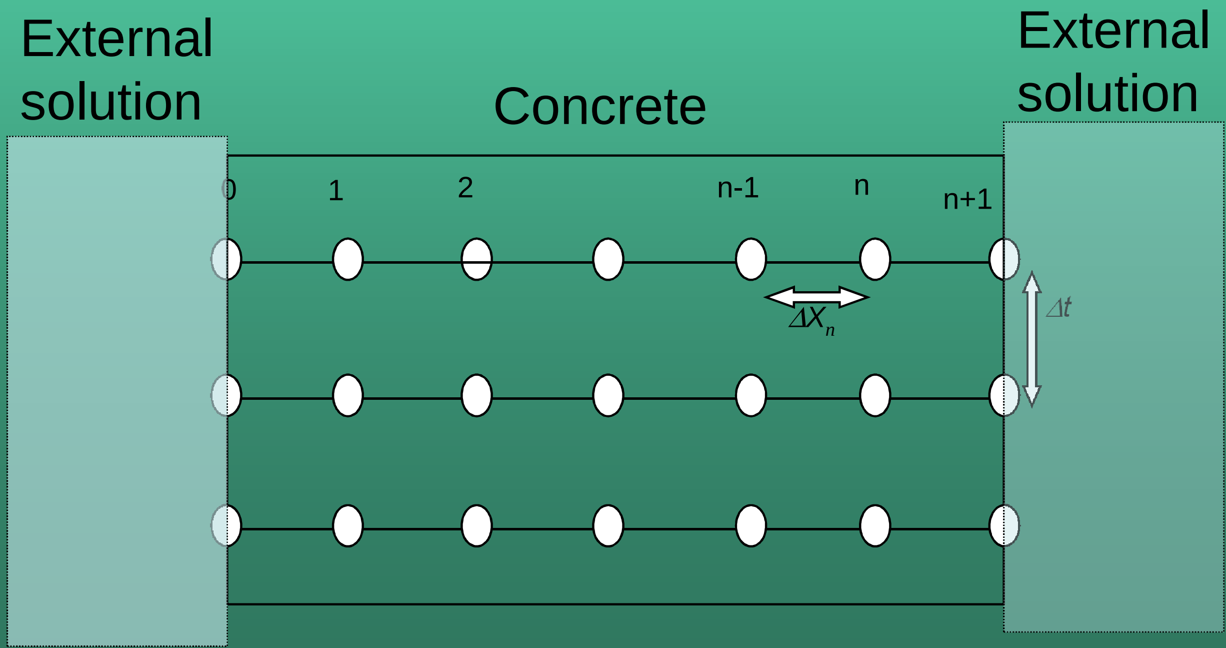
- **Nernst-Planck equation:**

$$J_i = D_i \frac{\partial c_i}{\partial x} + \frac{z_i F}{RT} D_i c_i \frac{\partial E}{\partial x}$$

Diffusion **Migration**

- **Charge electroneutrality (Kirchoff's law):**

$$0 = F \sum_i z_i J_i$$



Definitions

- Multi-species
- Binding Capacity
- Pore Solution concentration

Definitions

C_l : free ions per unit volume of liquid
Cs: total ions per unit volume of the solid
α: binding capacity factor
ε: porosity

$$\alpha = \frac{C_s}{C_l}$$

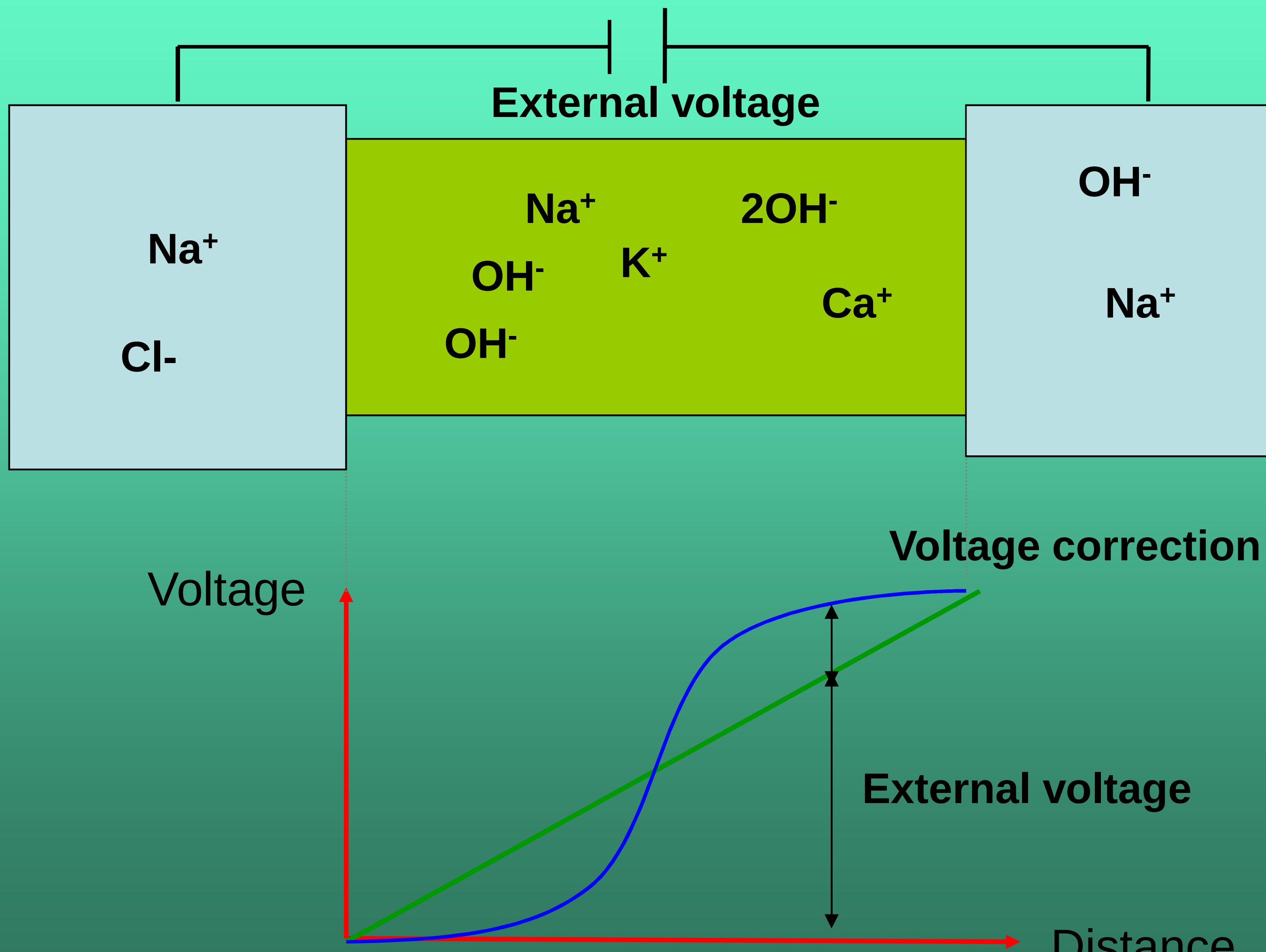
$$F = D_{app} \frac{dC_s}{dx}$$

The flux is calculated per unit area of the porous material and the average concentration in the material

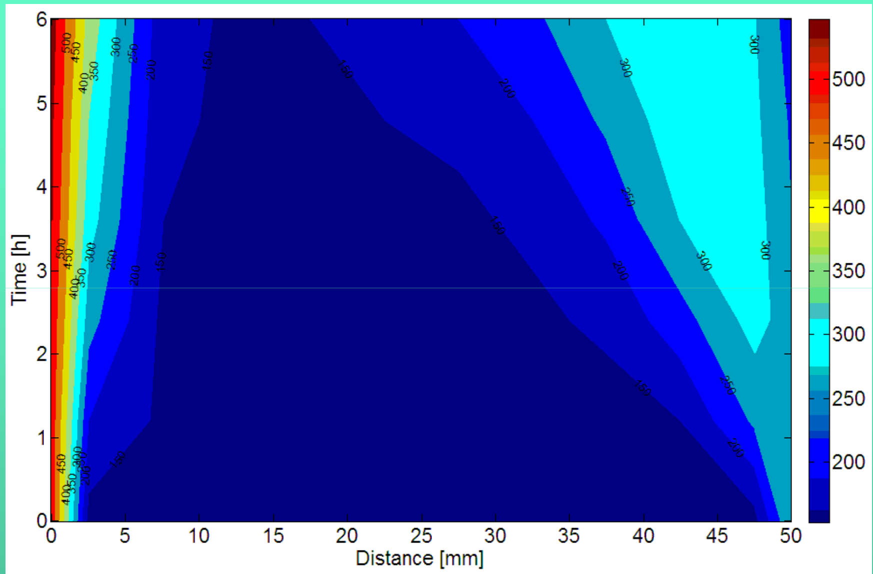
$$F = \varepsilon D_i \frac{dC_l}{dx}$$

The flux is calculated per unit cross-sectional area of the pores and the concentration in the free liquid

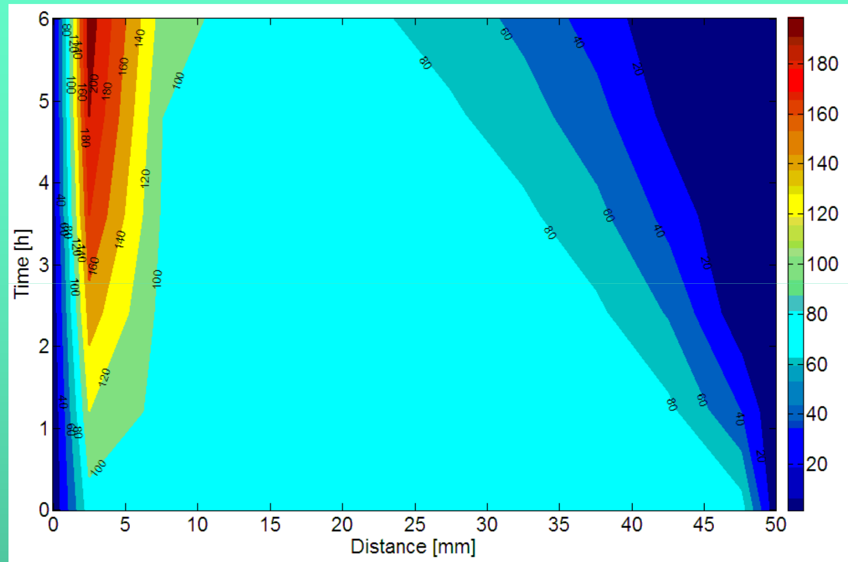
$$\frac{\alpha}{\varepsilon} = \frac{D_i}{D_{app}}$$


External voltage
Na+
Cl-
Na+
2OH-
OH-
K+
Ca+
OH-
OH-
Na+
Voltage correction
Voltage
External voltage
Distance

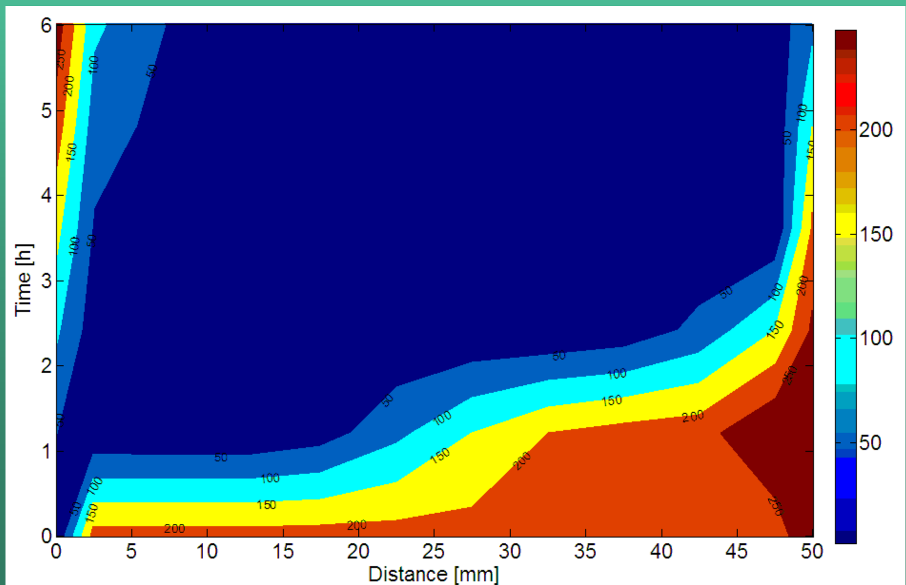
Numerical Model



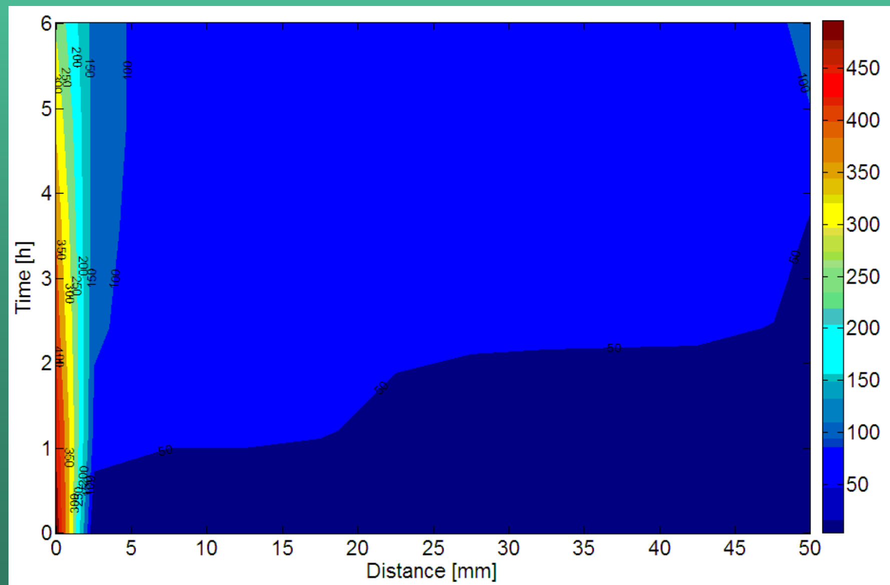
Concentration Na [mol/m3]



Concentration K [mol/m3]



Concentration OH [mol/m3]



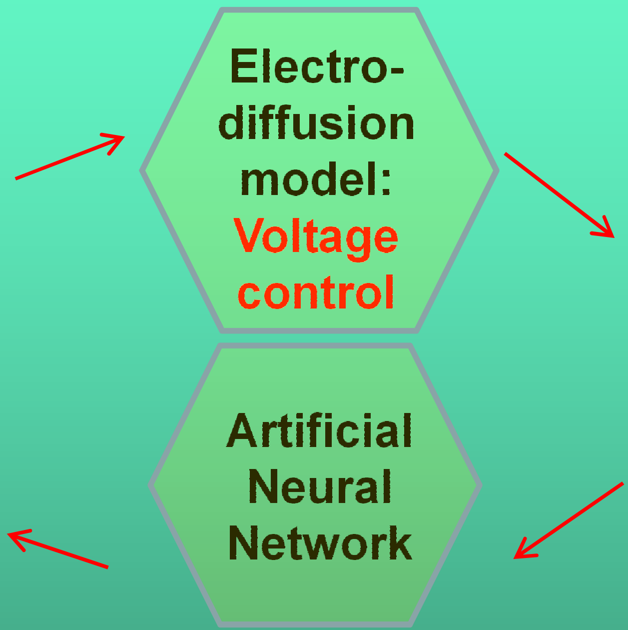
Concentration Cl [mol/m3]

Optimization Model

Data base

Transport properties

- Intrinsic diffusion coefficient (Cl^-)
- Intrinsic diffusion coefficient (OH^-)
- Intrinsic diffusion coefficient (Na^+)
- Intrinsic diffusion coefficient (K^+)
- Porosity (ε)
- Chloride binding capacity factor (α)
- OH^- conc. of the pore solution



Experiments

- Current
- Membrane potential

Network training

References

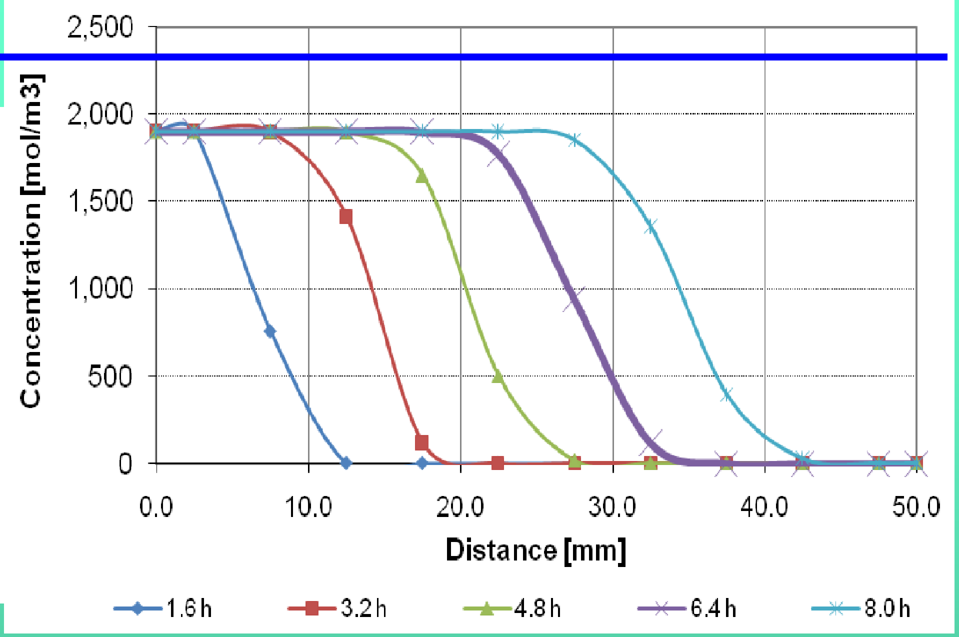
J. Lizarazo-Marriaga and P. Claisse, Determination of the transport properties of a blended concrete from its electrical properties measured during a migration test. **Magazine of Concrete Research**

Lizarazo-Marriaga and P. Claisse, Determination of the concrete chloride diffusion coefficient based on an electrochemical test and an optimization model. **Materials Chemistry and Physics**

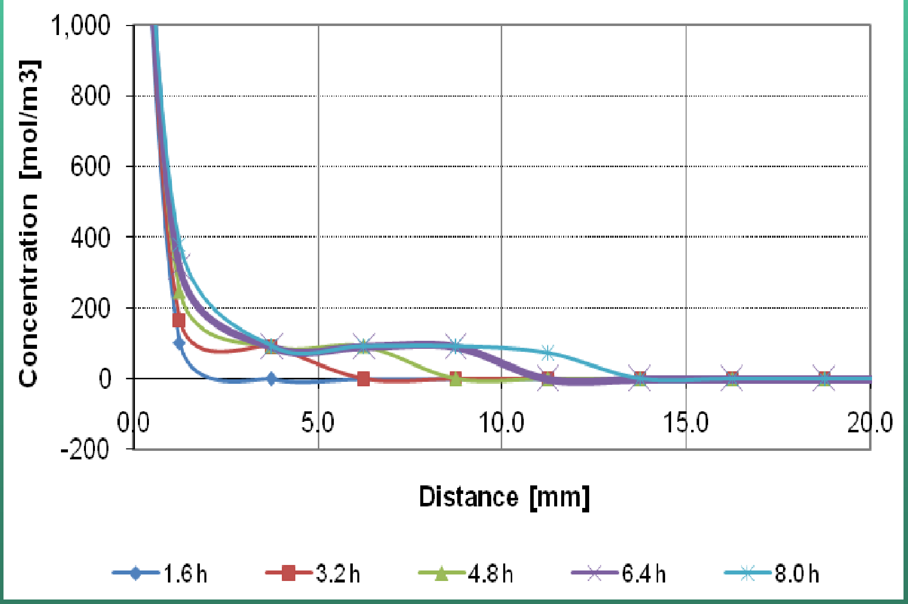
SIMULATION OF THE CONCRETE CHLORIDE NT BUILD-492 MIGRATION TEST

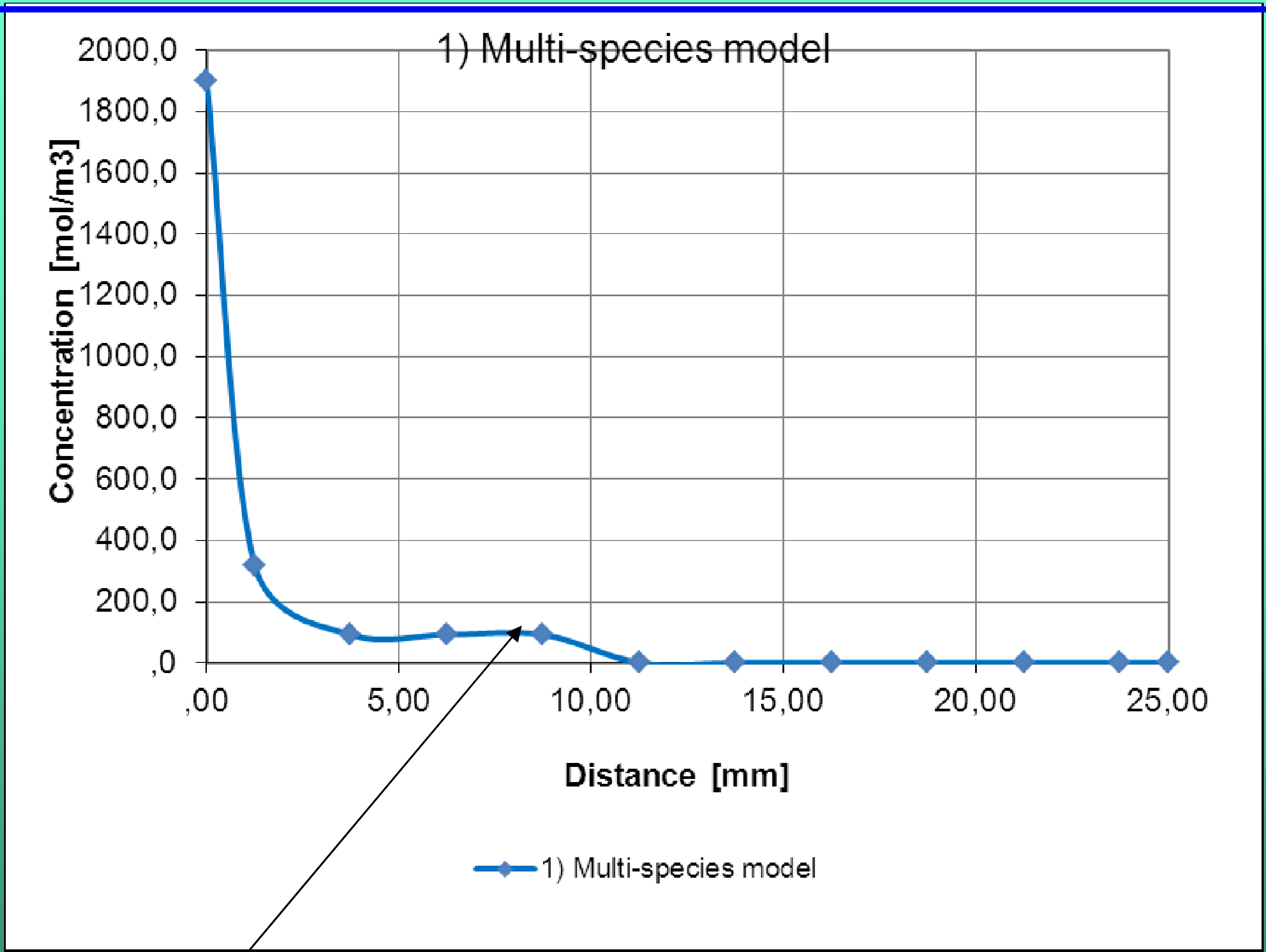
J. Lizarazo-Marriaga – P. Claisse – J. Gonzalez

	Valence z	Intrinsic Diffusion D m²/s	Concentration [mol/m³] (in liquid) negative	in sample	positive	Capacity factor
Chloride	-1	1.90×10^{-10}	1900	0.00E+00	0	1
No of cells:	500		Sample length [m]	0.05		
Voltage correction?	**NO**		Sample radius [m]	0.05		
Time step [s]:	1		Room temp [K]	295		
Run time [hours]:	8		Cell volumes [m³]:	1		
Porosity:	1		Heat loss fact [J/K]:	0.3		
Applied voltage [V]:	8					



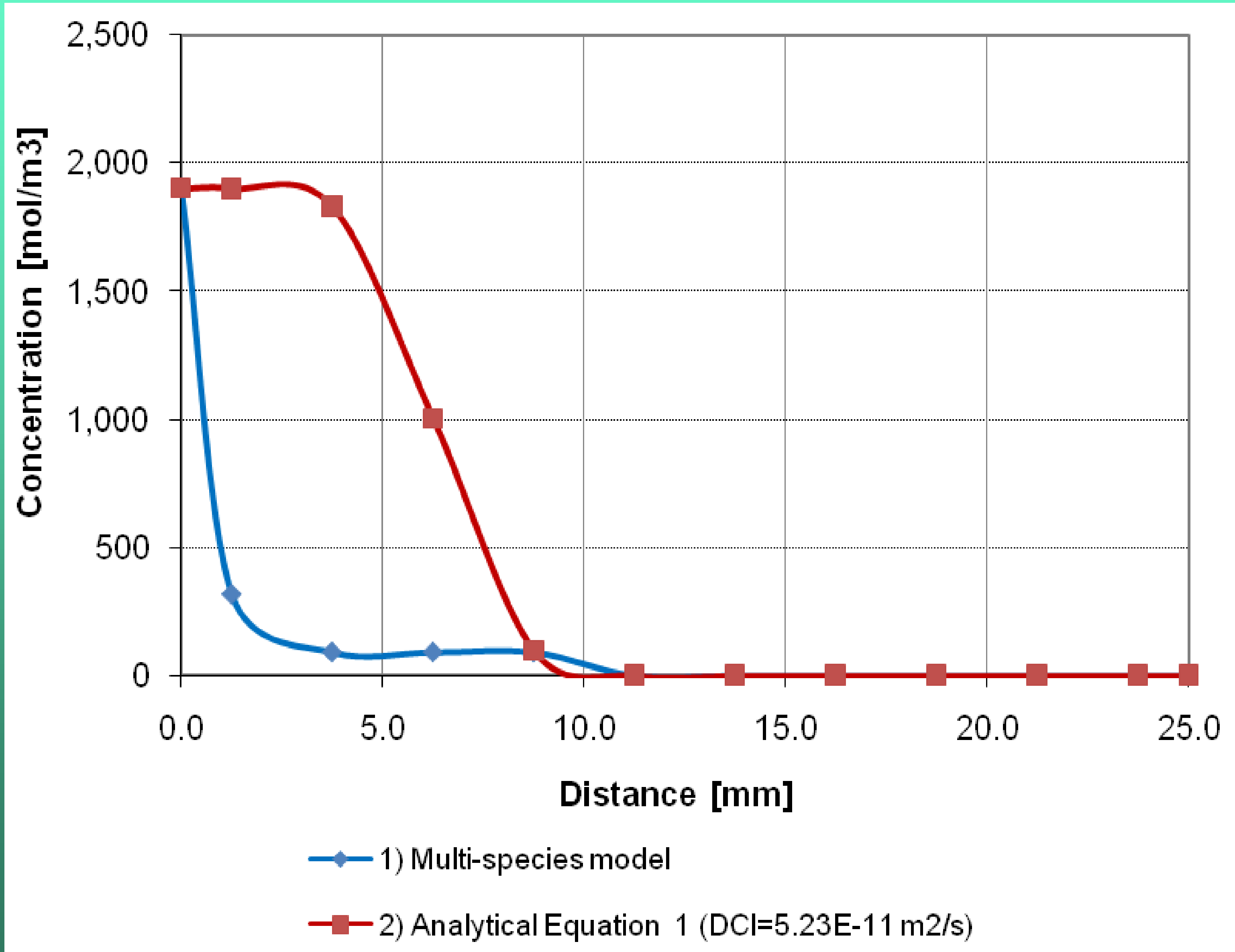
	Valence Z	Intrinsic Diffusion D m²/s	Concentration [mol/m³] (in liquid) negative	in sample	positive	Capacity factor
hydroxyl	-1	7.877E-11	0	239.973	300	0.171
chloride	-1	1.904E-10	1900	0.00E+00	0	0.383
sodium	1	2.061E-11	1900	7.92E+01	300	0.171
potassium	1	4.099E-12	0	1.61E+02	0	0.171
No of cells:	500		Sample length [m]	0.05		
Voltage correction?	**YES**		Sample radius [m]	0.05		
Time step [s]:	1		Room temperature [K]	295		
Run time [hours]:	8		Cell volumes [m³]:	0.03		
Porosity:	0.171		Heat loss factor [J/K]:	0.30		
Applied voltage [V]:	8					





chloride profile at 6.4 hours had a penetration of 9.3 mm when the concentration was 70 mol/m3

The chloride profile at 6.4 hours had a penetration of 9.3 mm when the concentration was 70 mol/m3



Thanks