



Modelado en COMSOL Multiphysics de un proceso de microscopía electrónica en fase líquida

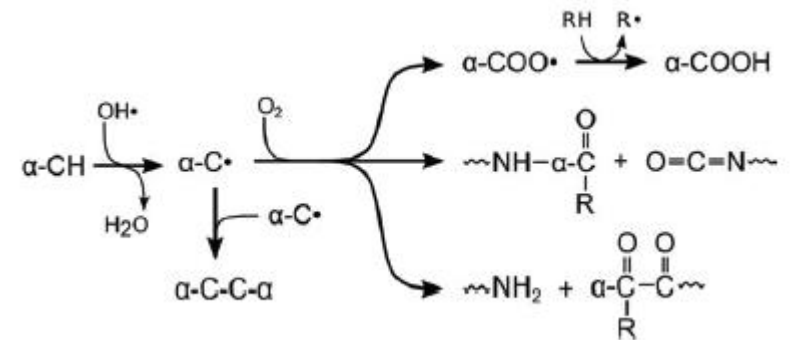
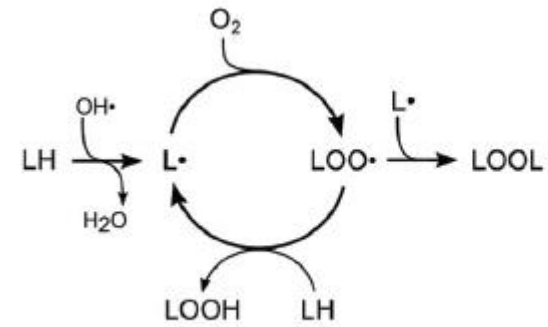
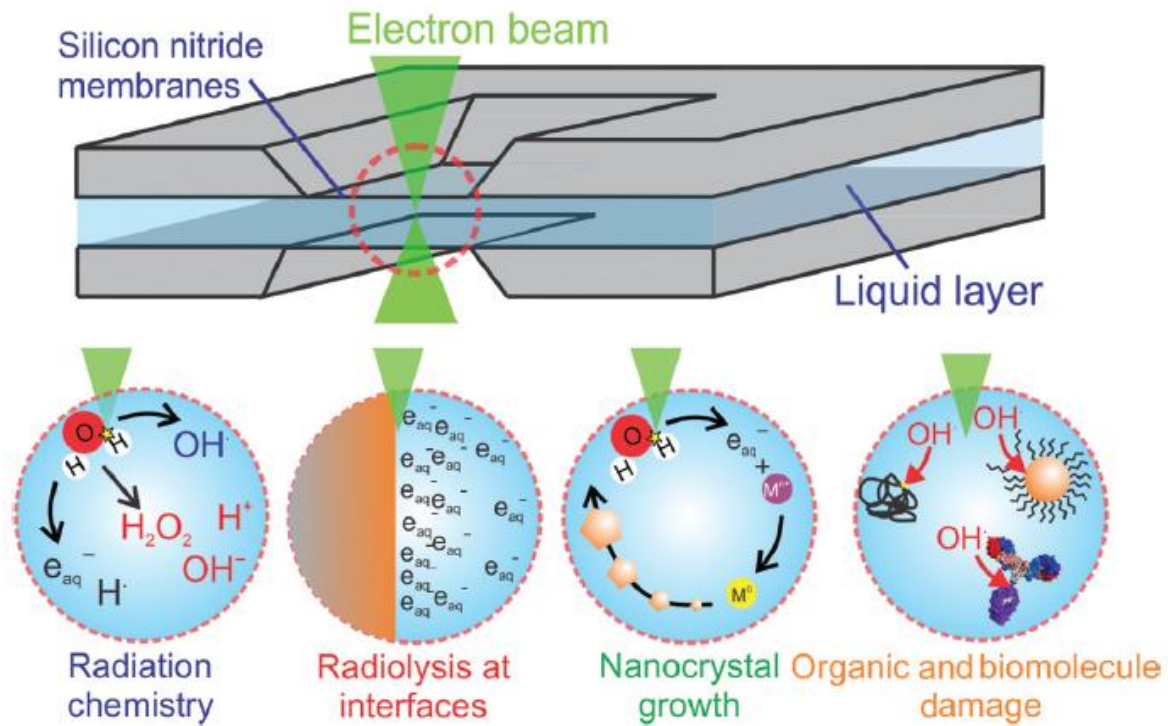
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(Curso académico 2020/2021)

Introducción y fundamento teórico:



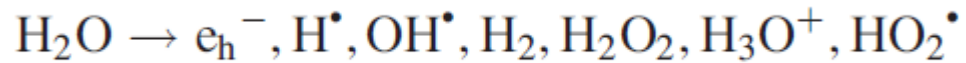
Introducción y fundamento teórico:

Reaction #	Equilibria	pK _a (25°C)
2	$H_2O \leftrightarrow H^+ + OH^-$	13.999
3	$H_2O_2 \leftrightarrow H^+ + HO_2^-$	11.65
4	$OH \leftrightarrow H^+ + O^-$	11.9
5	$HO_2 \leftrightarrow H^+ + O_2^-$	4.57
6	$H \leftrightarrow H^+ + e_{aq}^-$	9.77
	Chemical Reaction	Rate Constant (25°C) (M ⁻¹ s ⁻¹ unless specified otherwise)
7	$H^+ + OH^- \rightarrow H_2O$	1.4×10^{11}
8	$H_2O \rightarrow H^+ + OH^-$	$\frac{k_7 \times K_2}{[H_2O]} s^{-1}$
9	$H_2O_2 \rightarrow H^+ + HO_2^-$	$k_{10} \times K_3 s^{-1}$
10	$H^+ + HO_2^- \rightarrow H_2O_2$	5.0×10^{10}
11	$H_2O_2 + OH^- \rightarrow HO_2^- + H_2O$	1.3×10^{10}
12	$HO_2^- + H_2O \rightarrow H_2O_2 + OH^-$	$\frac{k_{11} \times K_2}{K_3 \times [H_2O]}$
13	$e_{aq}^- + H_2O \rightarrow H + OH^-$	1.9×10^7
14	$H + OH^- \rightarrow e_{aq}^- + H_2O$	2.2×10^7
15	$H \rightarrow e_{aq}^- + H^+$	$k_{16} \times K_6 s^{-1}$
16	$e_{aq}^- + H^+ \rightarrow H$	2.3×10^{10}
17	$OH + OH^- \rightarrow O^- + H_2O$	1.3×10^{10}
18	$O^- + H_2O \rightarrow OH + OH^-$	$\frac{k_{17} \times K_2}{K_4 \times [H_2O]}$
19	$OH \rightarrow O^- + H^+$	$k_{20} \times K_4 s^{-1}$
20	$O^- + H^+ \rightarrow OH$	1.0×10^{11}
21	$HO_2 \rightarrow O_2^- + H^+$	$k_{22} \times K_5 s^{-1}$
22	$O_2^- + H^+ \rightarrow HO_2$	5.0×10^{10}
23	$HO_2 + OH^- \rightarrow O_2^- + H_2O$	5.0×10^{10}
24	$O_2^- + H_2O \rightarrow HO_2 + OH^-$	$\frac{k_{23} \times K_2}{K_5 \times [H_2O]}$
25	$e_{aq}^- + OH \rightarrow OH^-$	3.0×10^{10}
26	$e_{aq}^- + H_2O_2 \rightarrow OH + OH^-$	1.1×10^{10}
27	$e_{aq}^- + O_2^- + H_2O \rightarrow HO_2^- + OH^-$	$\frac{1.3 \times 10^{10}}{[H_2O]} M^{-2} s^{-1}$
28	$e_{aq}^- + HO_2 \rightarrow HO_2^-$	2.0×10^{10}
29	$e_{aq}^- + O_2 \rightarrow O_2^-$	1.9×10^{10}
30	$e_{aq}^- + e_{aq}^- + 2H_2O \rightarrow H_2 + 2OH^-$	$\frac{5.5 \times 10^9}{[H_2O]^2} M^{-3} s^{-1}$
31	$e_{aq}^- + H + H_2O \rightarrow H_2 + OH^-$	$\frac{2.5 \times 10^{10}}{[H_2O]} M^{-2} s^{-1}$
32	$e_{aq}^- + HO_2 \rightarrow O^- + OH^-$	3.5×10^9
33	$e_{aq}^- + O^- + H_2O \rightarrow OH^- + OH^-$	$\frac{2.2 \times 10^{10}}{[H_2O]} M^{-2} s^{-1}$
34	$e_{aq}^- + O_3^- + H_2O \rightarrow O_2 + OH^- + OH^-$	$\frac{1.6 \times 10^{10}}{[H_2O]} M^{-2} s^{-1}$
35	$e_{aq}^- + O_3 \rightarrow O_3^-$	3.6×10^{10}
36	$H + H_2O \rightarrow H_2 + OH$	1.1×10^1

37	$H + O^- \rightarrow OH^-$	1.0×10^{10}
38	$H + HO_2^- \rightarrow OH + OH^-$	9.0×10^7
39	$H + O_3^- \rightarrow OH^- + O_2$	1.0×10^{10}
40	$H + H \rightarrow H_2$	7.8×10^9
41	$H + OH \rightarrow H_2O$	7.0×10^9
42	$H + H_2O_2 \rightarrow OH + H_2O$	9.0×10^7
43	$H + O_2 \rightarrow HO_2$	2.1×10^{10}
44	$H + HO_2 \rightarrow H_2O_2$	1.8×10^{10}
45	$H + O_2^- \rightarrow HO_2^-$	1.8×10^{10}
46	$H + O_3 \rightarrow HO_3$	3.8×10^{10}
47	$OH + OH \rightarrow H_2O_2$	3.6×10^9
48	$OH + HO_2 \rightarrow H_2O + O_2$	6.0×10^9
49	$OH + O_2^- \rightarrow OH^- + O_2$	8.2×10^9
50	$OH + H_2 \rightarrow H + H_2O$	4.3×10^7
51	$OH + H_2O_2 \rightarrow HO_2 + H_2O$	2.7×10^7
52	$OH + O^- \rightarrow HO_2^-$	2.5×10^{10}
53	$OH + HO_2^- \rightarrow HO_2 + OH^-$	7.5×10^9
54	$OH + O_3^- \rightarrow O_3 + OH^-$	2.6×10^9
55	$OH + O_3 \rightarrow O_2^- + O_2 + H^+$	6.0×10^9
56	$OH + O_3 \rightarrow HO_2 + O_2$	1.1×10^8
57	$HO_2 + O_2^- \rightarrow HO_2^- + O_2$	8.0×10^7
58	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	7.0×10^5
59	$HO_2 + O^- \rightarrow O_2 + OH^-$	6.0×10^9
60	$HO_2 + H_2O_2 \rightarrow OH + O_2 + H_2O$	5.0×10^{-1}
61	$HO_2 + HO_2^- \rightarrow OH + O_2 + OH^-$	5.0×10^{-1}
62	$HO_2 + O_3^- \rightarrow O_2 + O_2 + OH^-$	6.0×10^9
63	$HO_2 + O_3 \rightarrow HO_3 + O_2$	5.0×10^8
64	$O_2^- + O_2^- + 2H_2O \rightarrow H_2O_2 + O_2 + 2OH^-$	$\frac{1.0 \times 10^7}{[H_2O]^2} M^{-3} s^{-1}$
65	$O_2^- + O^- + H_2O \rightarrow O_2 + 2OH^-$	$\frac{6.0 \times 10^4}{[H_2O]} M^{-2} s^{-1}$
66	$O_2^- + H_2O_2 \rightarrow OH + O_2 + OH^-$	1.3×10^{-1}
67	$O_2^- + HO_2^- \rightarrow O^- + O_2 + OH^-$	1.3×10^{-1}
68	$O_2^- + O_3^- + H_2O \rightarrow O_2 + O_2 + 2OH^-$	$\frac{1.0 \times 10^4}{[H_2O]} M^{-2} s^{-1}$
69	$O_2^- + O_3 \rightarrow O_3^- + O_2$	1.5×10^9
70	$O^- + O^- + H_2O \rightarrow HO_2^- + OH^-$	$\frac{1.0 \times 10^9}{[H_2O]} M^{-2} s^{-1}$
71	$O^- + O_2 \rightarrow O_3^-$	3.6×10^9
72	$O^- + H_2 \rightarrow H + OH^-$	8.0×10^7
73	$O^- + H_2O_2 \rightarrow O_2^- + H_2O$	5.0×10^8
74	$O^- + HO_2^- \rightarrow O_2^- + OH^-$	4.0×10^8
75	$O^- + O_3^- \rightarrow O_2 + O_2^-$	7.0×10^8
76	$O^- + O_3 \rightarrow O_2^- + O_2$	5.0×10^9
77	$O_3^- \rightarrow O_2 + O^-$	$3.3 \times 10^3 s^{-1}$
78	$O_3^- + H^+ \rightarrow O_2 + OH$	9.0×10^{10}
79	$HO_3 \rightarrow O_2 + OH$	$1.1 \times 10^5 s^{-1}$

Introducción y fundamento teórico:

- **Productos primarios debidos a la radiación:**

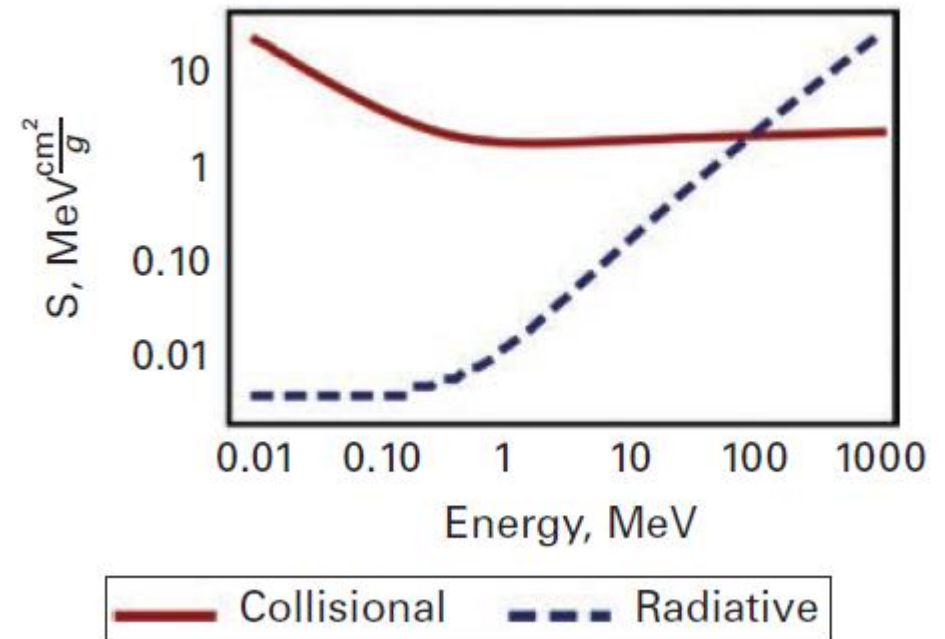


- **Energía perdida por el electrón y su dose rate:**

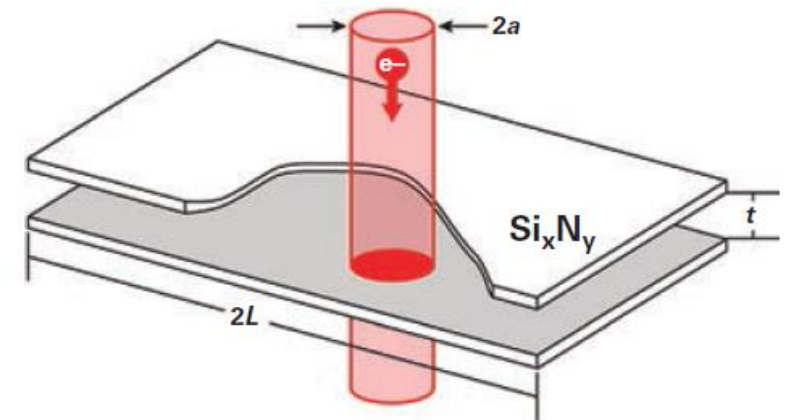
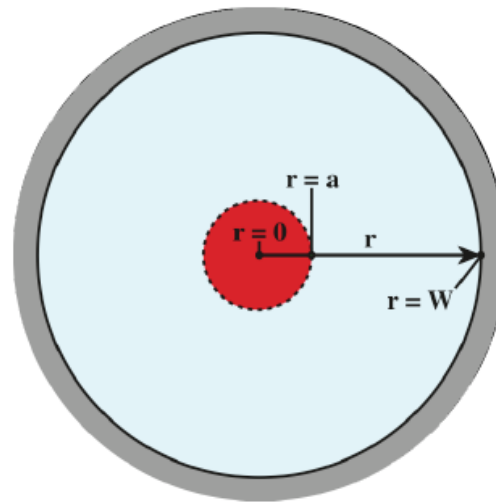
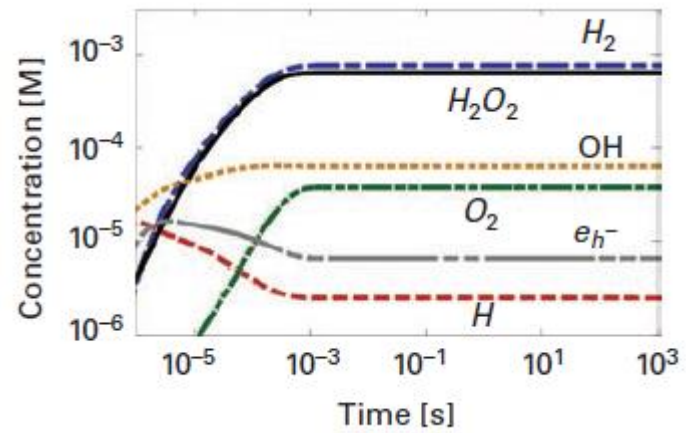
$$S_{\text{Total}} = \frac{dE}{ds} = S_R + S_C = \rho S \quad \psi = \frac{10^5 SI}{\pi a^2} \text{ (Gy/s)}$$

- **Ecuación de la concentración de las especies:**

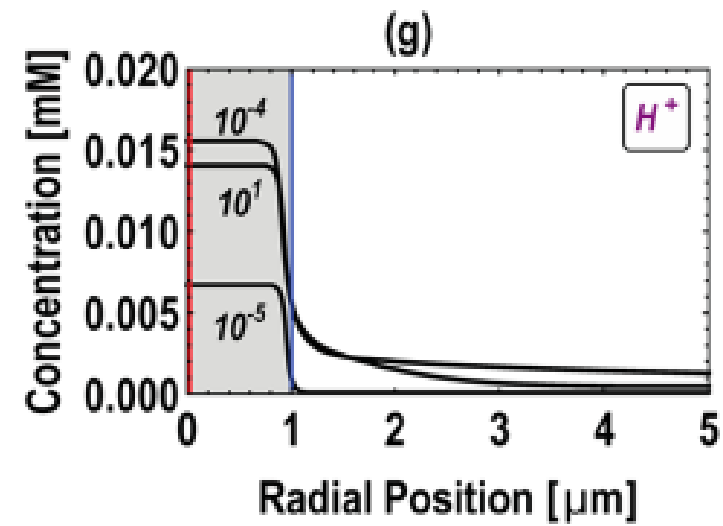
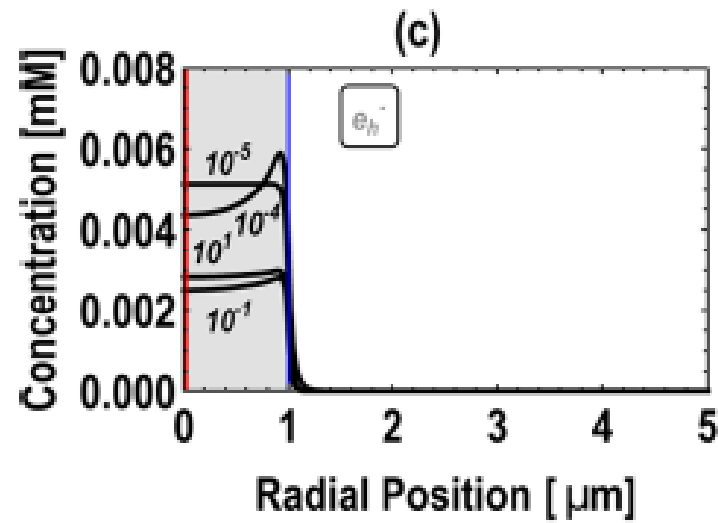
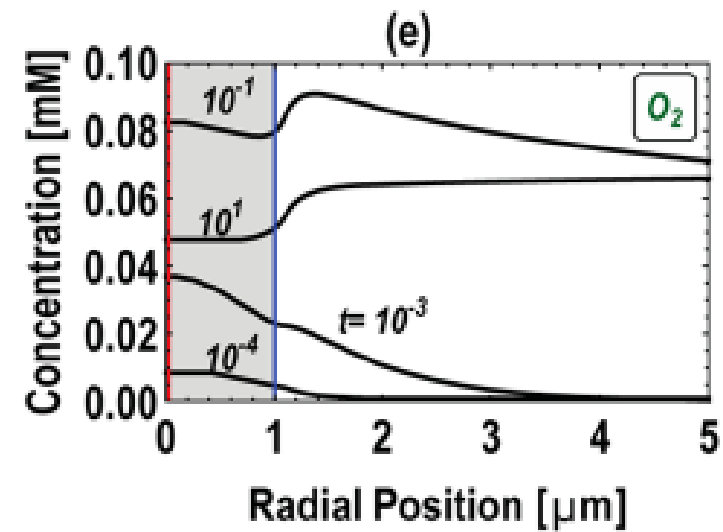
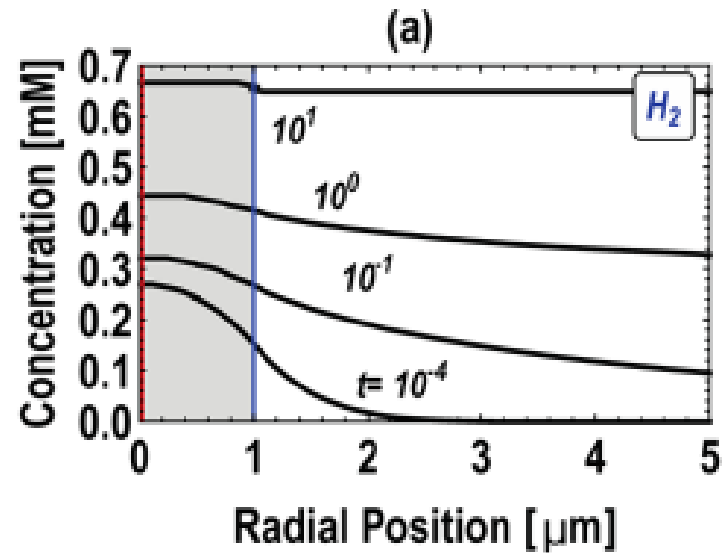
$$\frac{\partial C_i}{\partial t} = D_i \nabla^2 C_i - \sum_j k_{ij} C_i C_j + \sum_{j,k \neq i} k_{jk} C_j C_k + R_i$$



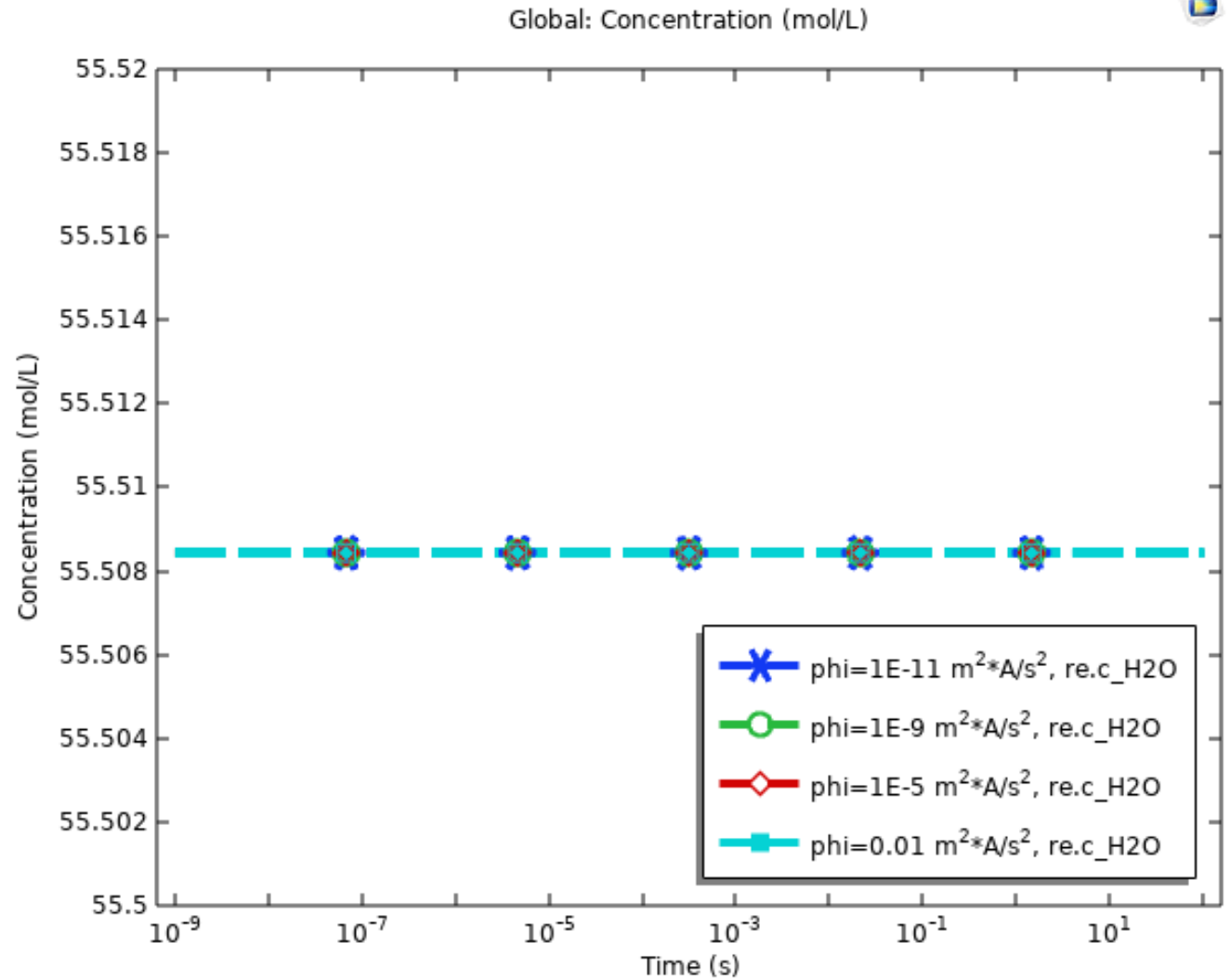
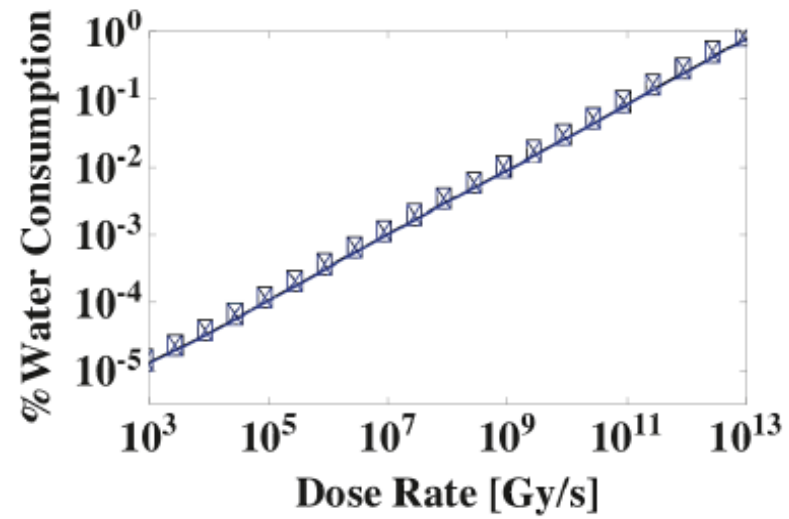
Introducción y fundamento teórico:



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Simplificaciones del problema:



Definiciones globales, parámetros:

Name	Expression	Value	Description
phi	$(S^*)/(\pi \cdot a^2)$	1.02E-11 m ² .A/s ²	Doserate depending on following values
S	$2[(\text{MeV} \cdot \text{cm}^2)/(\text{g})]$	3.2044E-14 m ⁴ /s ²	Stopping power
I	1e-9[A]	1E-9 A	Current
a	1e-4[cm]	1E-6 m	Beam radius
F	F_const	96485 C/mol	Faraday constant
rho	0.997[g/cm ³]	997 kg/m ³	Density of water

Name	Expression	Value	Description
GEHn	2.701033709730987e7[uM/s]	27010 mol/(m ³ .s)	generation due to Gvalues
GH2O	$-(\text{GOHn} + 2 \cdot \text{GH2O2} + \text{GOH} + 2 \cdot \text{GHO2})$	-44213 mol/(m ³ .s)	
GH2	1.323272999003653e6[uM/s]	1323.3 mol/(m ³ .s)	
GHO2	6.227167054134840e5[uM/s]	622.72 mol/(m ³ .s)	
GOH	2.825577050813684e7[uM/s]	28256 mol/(m ³ .s)	
GH	7.783958817668550e6[uM/s]	7784 mol/(m ³ .s)	
GH2O2	3.658460644304218e6[uM/s]	3658.5 mol/(m ³ .s)	
GOHn	7.394760876785121e6[uM/s]	7394.8 mol/(m ³ .s)	
GHp	3.440509797409499e7[uM/s]	34405 mol/(m ³ .s)	

Name	Expression	Value	Description
K1	$10^{-13.999}[(\text{mol/L})^2]$	1.0023E-8 mol ² /m ⁶	equilibrium rate constants (1/Ms) or (1/M ² s)
K2	$10^{-11.65}[(\text{mol/L})]$	2.2387E-9 mol/m ³	
K3	$10^{-11.9}[(\text{mol/L})]$	1.2589E-9 mol/m ³	
K4	$10^{-4.57}[(\text{mol/L})]$	0.026915 mol/m ³	
K5	$10^{-9.77}[(\text{mol/L})]$	1.6982E-7 mol/m ³	

Name	Expression	Value	Description
REHn	0[mol/m ³]	0 mol/m ³	initial concentration micromolar/sec
RHp	1e-4[mol/m ³]	1E-4 mol/m ³	
ROHn	1e-4[mol/m ³]	1E-4 mol/m ³	
RH2O2	0[mol/m ³]	0 mol/m ³	
RHO2n	0[mol/m ³]	0 mol/m ³	
RH	0[mol/m ³]	0 mol/m ³	
ROH	0[mol/m ³]	0 mol/m ³	
ROn	0[mol/m ³]	0 mol/m ³	
RHO2	0[mol/m ³]	0 mol/m ³	
RO2n	0[mol/m ³]	0 mol/m ³	
RO2	0[mol/m ³]	0 mol/m ³	
RH2	0[mol/m ³]	0 mol/m ³	
RO3n	0[mol/m ³]	0 mol/m ³	
RO3	0[mol/m ³]	0 mol/m ³	
RHO3	0[mol/m ³]	0 mol/m ³	
RH2O	$(1000000/18.01528)[\text{mol/m}^3]$	55508 mol/m ³	

Interfaz física:

Model Builder

- TFM.mph (root)
 - Global Definitions
 - Parameters
 - initial concentration mol/m³
 - Rate constants (1/Ms) or (1/M²s); a
 - Equilibrium rate constants (1/Ms) or (
 - Generation due to G-values
 - Generation due to G-values Schneide
 - Gvalues at 300 KeV (Hill &Smith)
 - Materials
 - Component 1 (comp1)
 - Definitions
 - Reaction Engineering (re)
 - Initial Values 1
 - Additional Source due to Gvalues
 - Additional Source due to G-value
 - Species
 - Reversible reactions
 - Irreversible reactions
 - EHn reactions
 - H reactions
 - OH reactions
 - HO2 reactions
 - O2n reactions
 - On reactions
 - Equation View

Settings

Reaction Engineering

Label: Reaction Engineering

Name: re

Equation

Reactor

Reactor type: Batch, constant volume

Mass balance

Reactor volume: V_r 1[m³] m³

Energy Balance

Exclude

Temperature: T 293.15[K] K

Mixture Properties

Thermodynamics

Phase: Liquid

Calculate Transport Properties

Reaction

Label: 2: H2O2<=>Hp+HO2n

Reaction Formula Balance

Formula: H2O2<=>Hp+HO2n Apply

Reaction type: Reversible

$$R_i = \sum_j \nu_{ij} r_j$$

Reaction Rate

User defined

Reaction rate: r_j re.kf_1*re.c_Hp*re. mol/(m³.s) Reset to Default

Volumetric overall reaction order

Forward: 2

Reverse: 1

Rate Constants

Specify equilibrium constant

Use Arrhenius expressions

Forward rate constant: k^f k1 m³/(s.mol)

Reverse rate constant: k^r 0 1/s

Reaction Formula Balance

Formula: OH+OHn=>On+H2O Apply

Reaction type: Irreversible

$$R_i = \sum_j \nu_{ij} r_j$$

Reaction Rate

User defined

Reaction rate: r_j re.kf_23*re.c_OH*r. mol/(m³.s) Reset to Default

Volumetric overall reaction order

Forward: 2

Rate Constants

Use Arrhenius expressions

Forward rate constant: k^f k11 m³/(s.mol)

Interfaz física:

Reaction Engineering (re)

Initial Values 1

Reversible reactions

- 1: $\text{H}_p + \text{OH}_n \rightleftharpoons \text{H}_2\text{O}$
- 2: $\text{H}_2\text{O}_2 \rightleftharpoons \text{H}_p + \text{HO}_2n$
- 7: $\text{H}_2\text{O}_2 + \text{OH}_n \rightleftharpoons \text{HO}_2n + \text{H}_2\text{O}$
- 5: $\text{EH}_n + \text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}_n$
- 6: $\text{H} \rightleftharpoons \text{H}_p + \text{EH}_n$
- 8: $\text{H} \rightleftharpoons \text{H}_p + \text{EH}_n$
- 9: $\text{OH} \rightleftharpoons \text{O}_n + \text{H}_p$
- 10: $\text{HO}_2 \rightleftharpoons \text{H}_p + \text{O}_2n$
- 11: $\text{HO}_2 + \text{OH}_n \rightleftharpoons \text{O}_2n + \text{H}_2\text{O}$
- 40: $\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$

H reactions

- 26: $\text{H} + \text{O}_n \rightleftharpoons \text{OH}_n$
- 27: $\text{H} + \text{HO}_2n \rightleftharpoons \text{OH} + \text{OH}_n$
- 28: $\text{H} + \text{O}_3n \rightleftharpoons \text{OH}_n + \text{O}_2$
- 29: $\text{H} + \text{H} \rightleftharpoons \text{H}_2$
- 30: $\text{H} + \text{OH} \rightleftharpoons \text{H}_2\text{O}$
- 31: $\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{OH} + \text{H}_2\text{O}$
- 32: $\text{H} + \text{O}_2 \rightleftharpoons \text{HO}_2$
- 33: $\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2$
- 34: $\text{H} + \text{O}_2n \rightleftharpoons \text{HO}_2n$
- 35: $\text{H} + \text{O}_3 \rightleftharpoons \text{HO}_3$

EHn reactions

- 12: $\text{EH}_n + \text{OH} \rightleftharpoons \text{OH}_n$
- 13: $\text{EH}_n + \text{H}_2\text{O}_2 \rightleftharpoons \text{OH} + \text{OH}_n$
- 14: $\text{EH}_n + \text{O}_2n \rightleftharpoons \text{HO}_2n + \text{OH}_n$
- 15: $\text{EH}_n + \text{HO}_2 \rightleftharpoons \text{HO}_2n$
- 16: $\text{EH}_n + \text{O}_2 \rightleftharpoons \text{O}_2n$
- 17: $\text{EH}_n + \text{EH}_n \rightleftharpoons \text{H}_2 + 2\text{OH}_n$
- 18: $\text{EH}_n + \text{H} \rightleftharpoons \text{H}_2 + \text{OH}_n$
- 19: $\text{EH}_n + \text{HO}_2n \rightleftharpoons \text{O}_n + \text{OH}_n$
- 20: $\text{EH}_n + \text{O}_n \rightleftharpoons \text{OH}_n + \text{OH}_n$
- 21: $\text{EH}_n + \text{O}_3n \rightleftharpoons \text{O}_2 + \text{OH}_n + \text{OH}_n$
- 22: $\text{EH}_n + \text{O}_3 \rightleftharpoons \text{O}_3n$

OH reactions

- 36: $\text{OH} + \text{OH} \rightleftharpoons \text{H}_2\text{O}_2$
- 37: $\text{OH} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$
- 38: $\text{OH} + \text{O}_2n \rightleftharpoons \text{OH}_n + \text{O}_2$
- 41: $\text{OH} + \text{H}_2\text{O}_2 \rightleftharpoons \text{HO}_2 + \text{H}_2\text{O}$
- 42: $\text{OH} + \text{O}_n \rightleftharpoons \text{HO}_2n$
- 43: $\text{OH} + \text{HO}_2n \rightleftharpoons \text{HO}_2 + \text{OH}_n$
- 44: $\text{OH} + \text{O}_3n \rightleftharpoons \text{O}_3 + \text{OH}_n$
- 45: $\text{OH} + \text{O}_3n \rightleftharpoons \text{O}_2n + \text{O}_2n + \text{H}_p$
- 46: $\text{OH} + \text{O}_3 \rightleftharpoons \text{HO}_2 + \text{O}_2$

O_n reactions

- 60: $\text{O}_n + \text{O}_n \rightleftharpoons \text{HO}_2n + \text{OH}_n$
- 61: $\text{O}_n + \text{O}_2 \rightleftharpoons \text{O}_3n$
- 62: $\text{O}_n + \text{H}_2 \rightleftharpoons \text{H} + \text{OH}_n$
- 63: $\text{O}_n + \text{H}_2\text{O}_2 \rightleftharpoons \text{O}_2n + \text{H}_2\text{O}$
- 64: $\text{O}_n + \text{HO}_2n \rightleftharpoons \text{O}_2n + \text{OH}_n$
- 65: $\text{O}_n + \text{O}_3n \rightleftharpoons \text{O}_2n + \text{O}_2n$
- 66: $\text{O}_n + \text{O}_3 \rightleftharpoons \text{O}_2n + \text{O}_2$

HO₂ reactions

- 47: $\text{HO}_2 + \text{O}_2n \rightleftharpoons \text{HO}_2n + \text{O}_2$
- 48: $\text{HO}_2 + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$
- 49: $\text{HO}_2 + \text{O}_n \rightleftharpoons \text{O}_2 + \text{OH}_n$
- 50: $\text{HO}_2 + \text{H}_2\text{O}_2 \rightleftharpoons \text{OH} + \text{O}_2 + \text{H}_2\text{O}$
- 51: $\text{HO}_2 + \text{HO}_2n \rightleftharpoons \text{OH} + \text{O}_2 + \text{OH}_n$
- 52: $\text{HO}_2 + \text{O}_3n \rightleftharpoons \text{O}_2 + \text{O}_2 + \text{OH}_n$
- 53: $\text{HO}_2 + \text{O}_3 \rightleftharpoons \text{HO}_3 + \text{O}_2$

Irreversible reactions

- 23: $\text{OH} + \text{OH}_n \rightleftharpoons \text{O}_n + \text{H}_2\text{O}$
- 24: $\text{O}_n \rightleftharpoons \text{OH} + \text{OH}_n$
- 67: $\text{O}_3n \rightleftharpoons \text{O}_2 + \text{O}_n$
- 68: $\text{O}_3n + \text{H}_p \rightleftharpoons \text{O}_2 + \text{OH}$
- 69: $\text{HO}_3 \rightleftharpoons \text{O}_2 + \text{OH}$

O_{2n} reactions

- 54: $\text{O}_2n + \text{O}_2n \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2 + 2\text{OH}_n$
- 55: $\text{O}_2n + \text{O}_n \rightleftharpoons \text{O}_2 + 2\text{OH}_n$
- 56: $\text{O}_2n + \text{H}_2\text{O}_2 \rightleftharpoons \text{OH} + \text{O}_2 + \text{OH}_n$
- 57: $\text{O}_2n + \text{HO}_2n \rightleftharpoons \text{O}_n + \text{O}_2 + \text{OH}_n$
- 58: $\text{O}_2n + \text{O}_3n \rightleftharpoons \text{O}_2 + \text{O}_2 + 2\text{OH}_n$
- 59: $\text{O}_2n + \text{O}_3 \rightleftharpoons \text{O}_3n + \text{O}_2$

Interfaz física:

The screenshot shows the 'Model Builder' window on the left and the 'Settings' panel on the right. The 'Species' folder is expanded, showing a list of species including 'Species: H2O'. The 'Settings' panel for 'Species: H2O' is visible, showing fields for 'Label', 'Equation', 'Species Name', 'Species Type', 'General Parameters', and 'Reaction Rate'.

Species Type

Bulk species

General Parameters

Charge:

z 0

Reaction Rate

$$R_i = \sum_j R_{ij} + R_{add,j}$$

User defined

Rate expression:

R_i mol/(m³.s)

Estudio y resoledor:

Settings

Time Dependent

Compute Update Solution

Label: Time Dependent

Study Settings

Time unit: s

Output times: $10^{\{\text{range}(\log_{10}(1.0\text{e-}9), 1/1000, \log_{10}(100))\}}$ s

Tolerance: Physics controlled

Results While Solving

Physics and Variables Selection

Modify model configuration for study step

Global Definitions

- Component 1 (comp1)
 - Definitions
 - Reaction Engineering (re)
 - Initial Values 1
 - Additional Source due to Gvalues Schneider
 - Additional Source due to G-values
 - Species
 - Reversible reactions
 - Irreversible reactions
 - EHn reactions
 - H reactions
 - OH reactions
 - HO2 reactions
 - O2n reactions
 - On reactions

Model Builder

- Component 1 (comp1)
 - G-Values
 - Parametric Sweep
 - Step 1: Time Dependent
 - Solver Configurations
 - Solution 1 (sol1)
 - Compile Equations: Time Dep
 - Dependent Variables 1
 - Time-Dependent Solver 1
 - Direct
 - Advanced
 - Fully Coupled 1
 - Parametric Solutions 1 (sol2)
 - phi=1E-11 (sol3)
 - phi=1E-9 (sol4)
 - phi=1E-5 (sol5)
 - phi=0.01 (sol6)
 - Job Configurations
 - Results
 - Datasets
 - Views
 - Derived Values
 - Tables
 - Agua como soluto G-values
 - Agua como disolvente
 - Agua como soluto a diferentes phi

Settings

Time-Dependent Solver

Compute to Selected Compute

Label: Time-Dependent Solver 1

General

Defined by study step: Step 1: Time Dependent

Time unit: s

Output times: $10^{\{\text{range}(\log_{10}(1.0\text{e-}9), 1/1000, \log_{10}(100))\}}$ s

Times to store: Steps taken by solver

Store every Nth step: 1

Relative tolerance: 1E-5

Absolute Tolerance

Time Stepping

Method: BDF

Steps taken by solver: Intermediate

Interpolate solution at end time

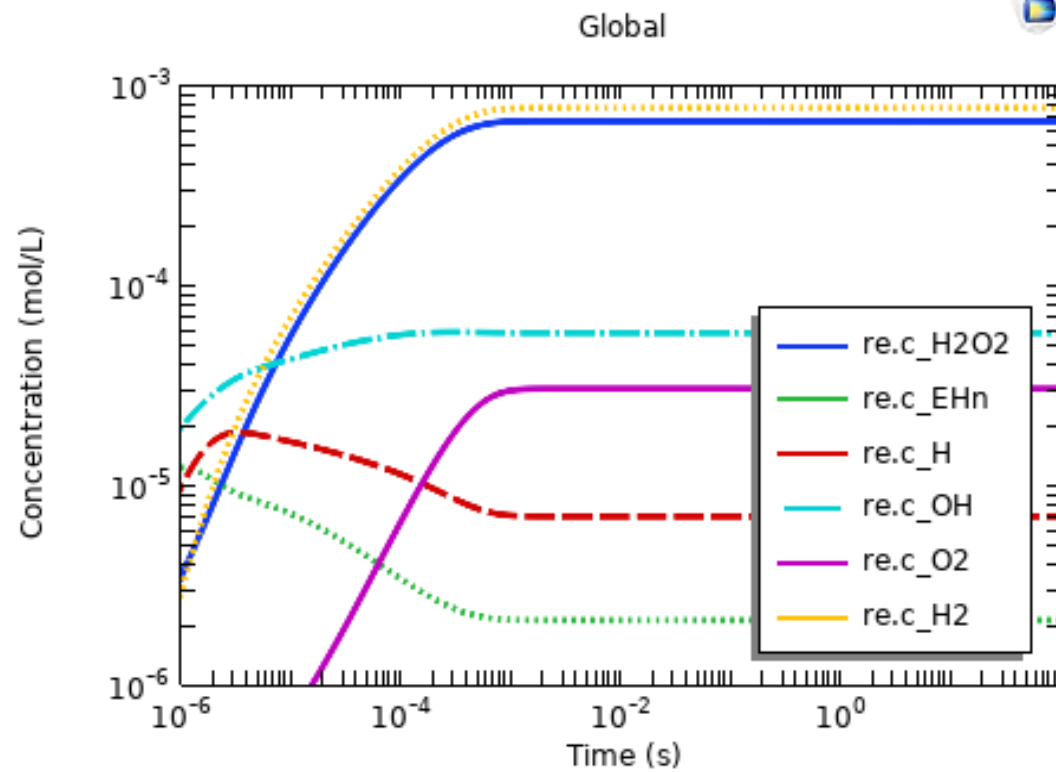
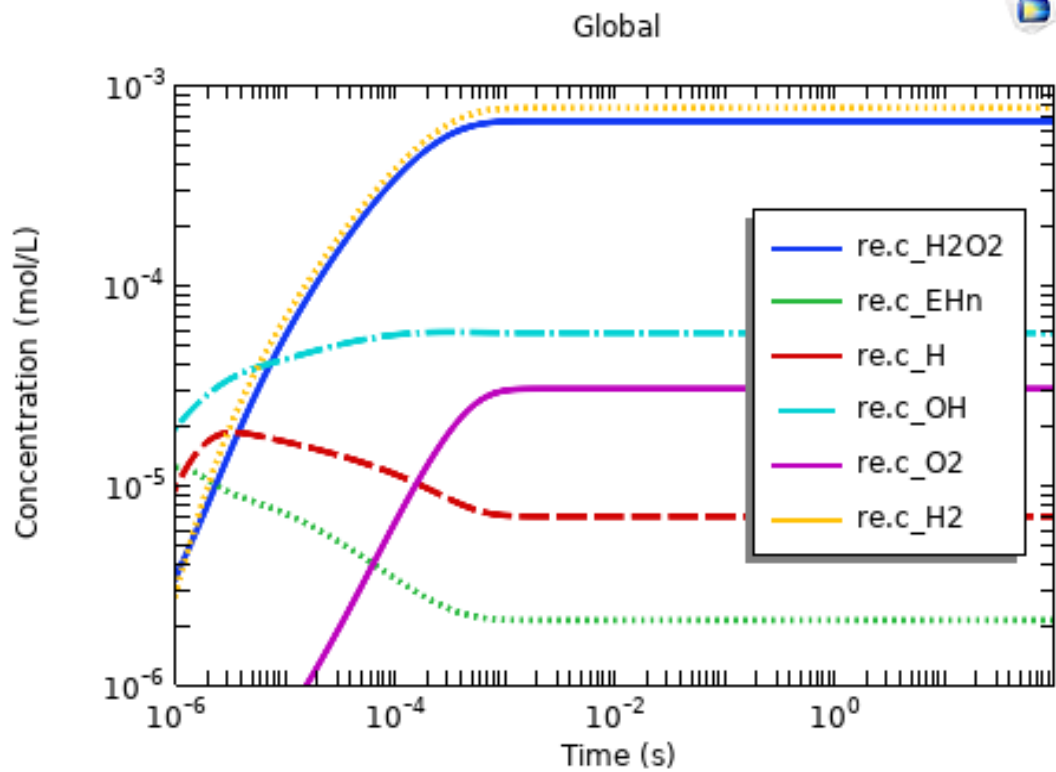
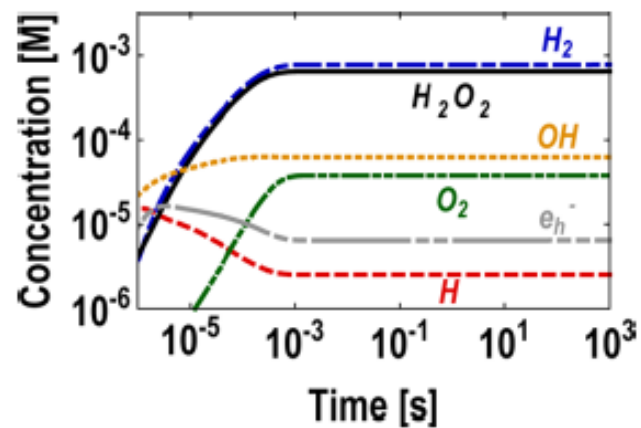
Initial step: 1e-9 s

Maximum step constraint: Automatic

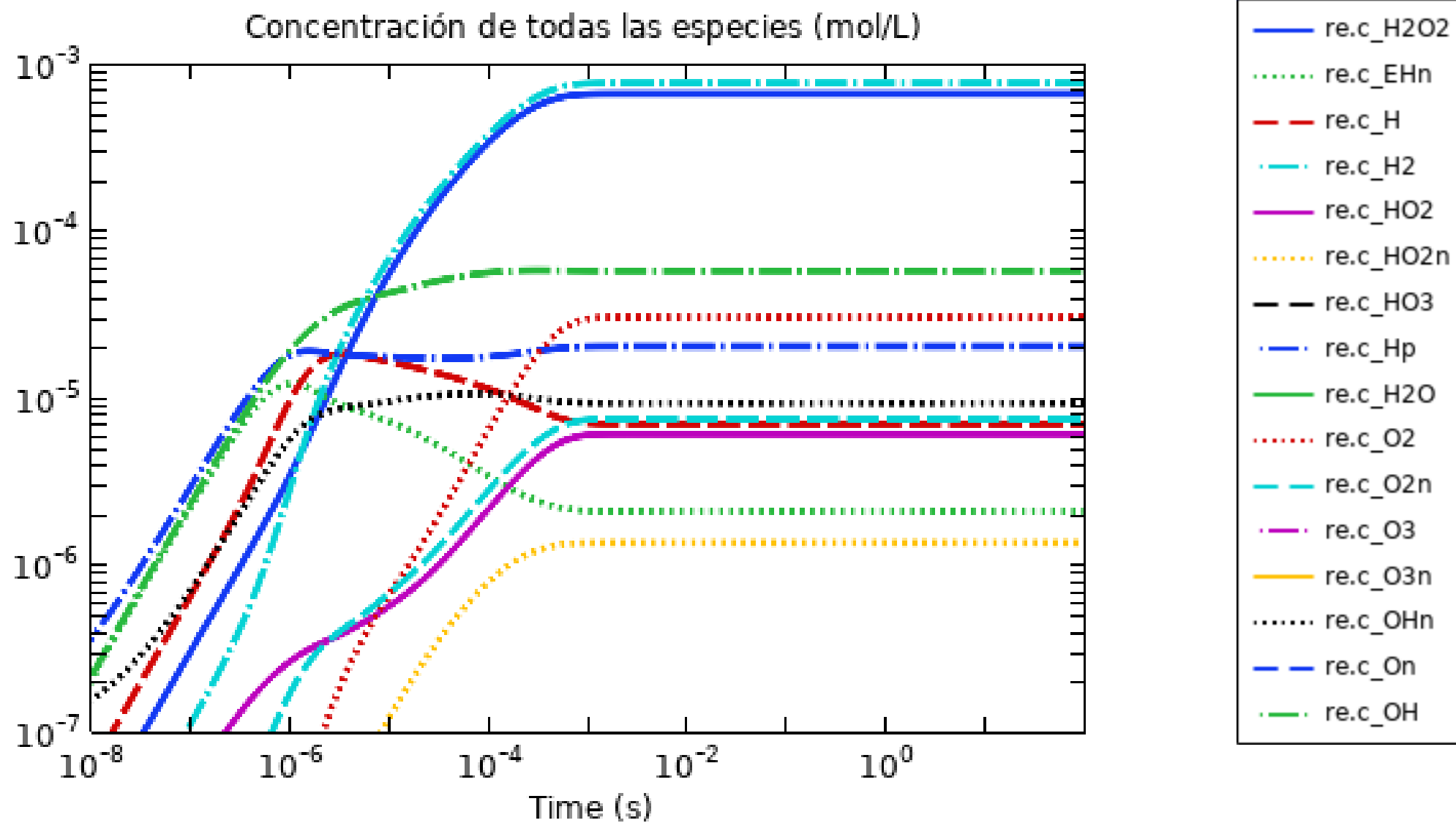
Maximum BDF order: 5

Minimum BDF order: 2

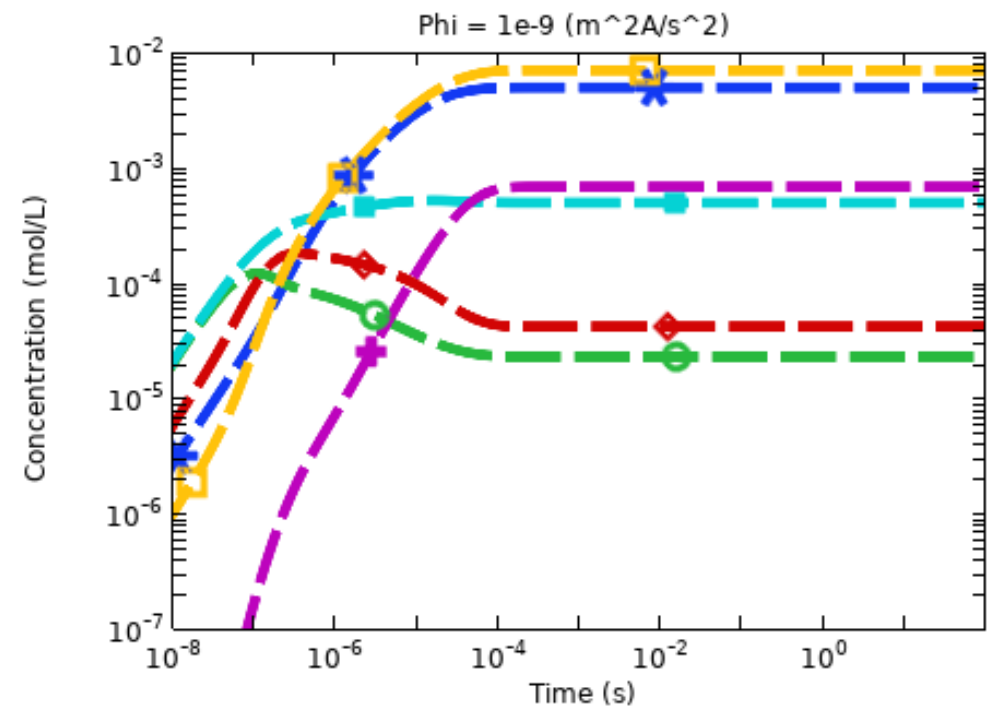
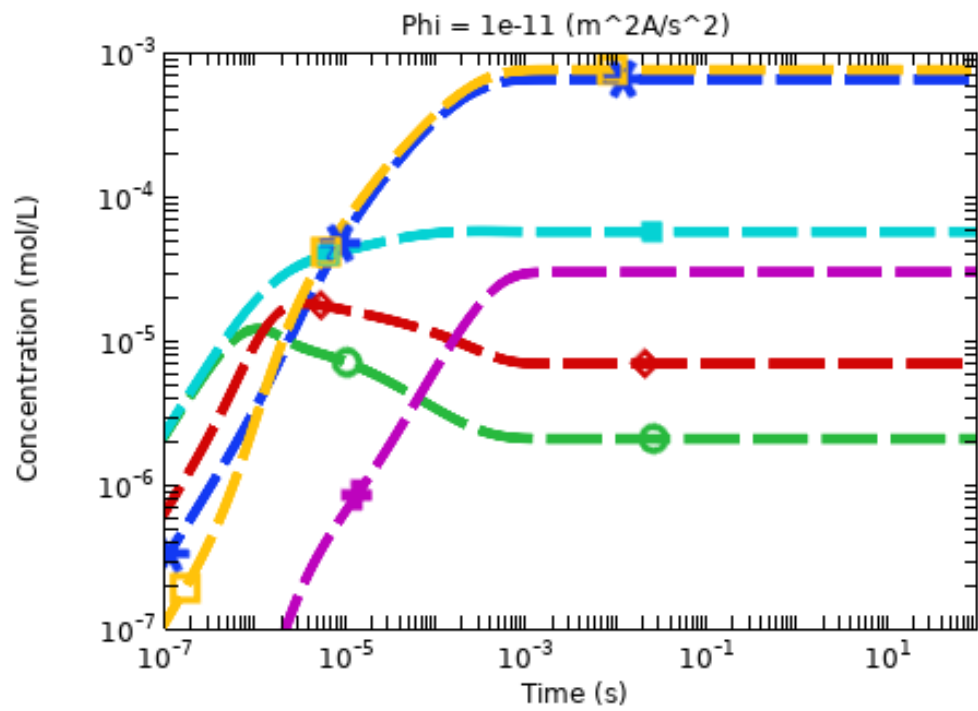
Resultados:



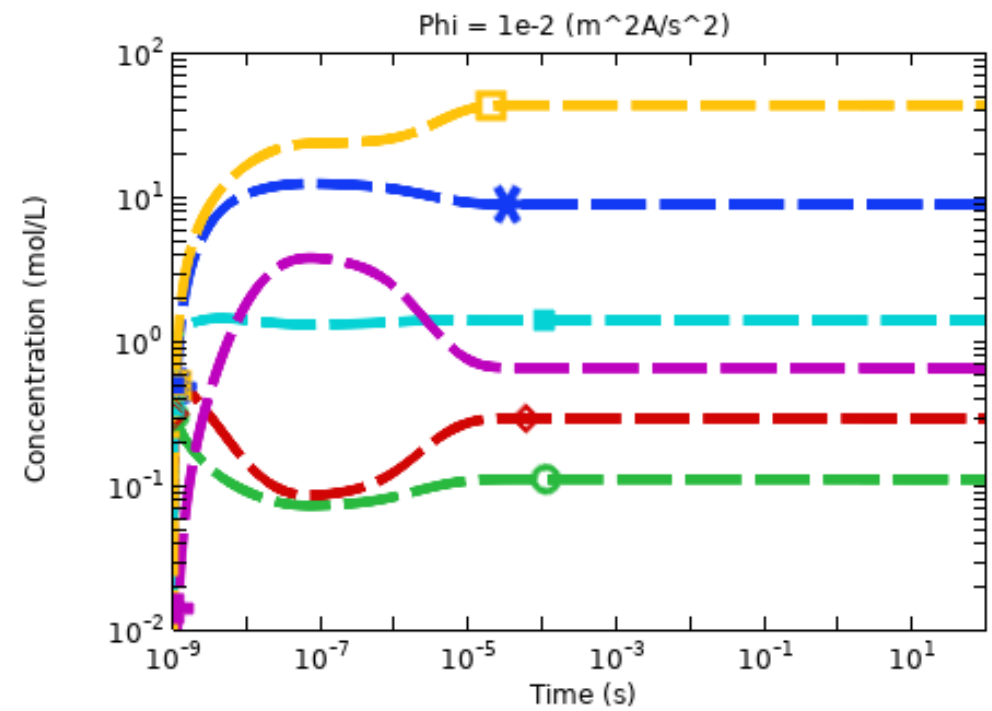
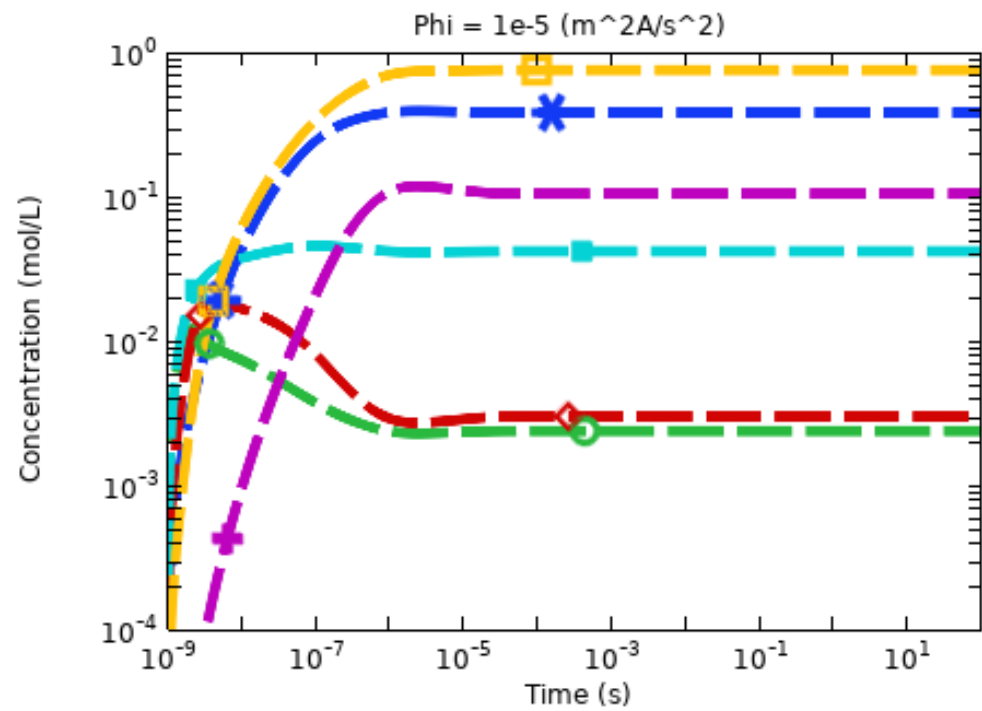
Resultados:



Resultados:



Resultados:



Conclusiones:

- **Reacciones casi instantáneas → Reactor tipo Bach.**
- **Aumentar el haz de electrones irradiado disminuye el tiempo al que se alcanza el estado estacionario y mayor velocidad cinética.**
- **Interesante ver cuales de las reacciones es más lenta y por tanto suprimible, asimismo cual es tan rápida que podemos tratar como una concentración inicial.**

Siguiente reto:

The screenshot shows the 'Model Builder' tab in COMSOL Multiphysics. A context menu is open over the 'Generate Space-Dependent Model' component. The menu items are:

- Reaction
- Species
- Reversible Reaction Group
- Equilibrium Reaction Group
- Parameter Estimation
- Additional Source
- Generate Space-Dependent Model
- Global Equations
- Global Constraint
- Weak Contribution
- Show More Options...
- Node Group
- Copy as Code to Clipboard
- Copy
- Delete
- Disable
- Disable in All Studies
- Rename
- Settings
- Properties
- Help

On the left, the 'Model Builder' tree shows the following structure:

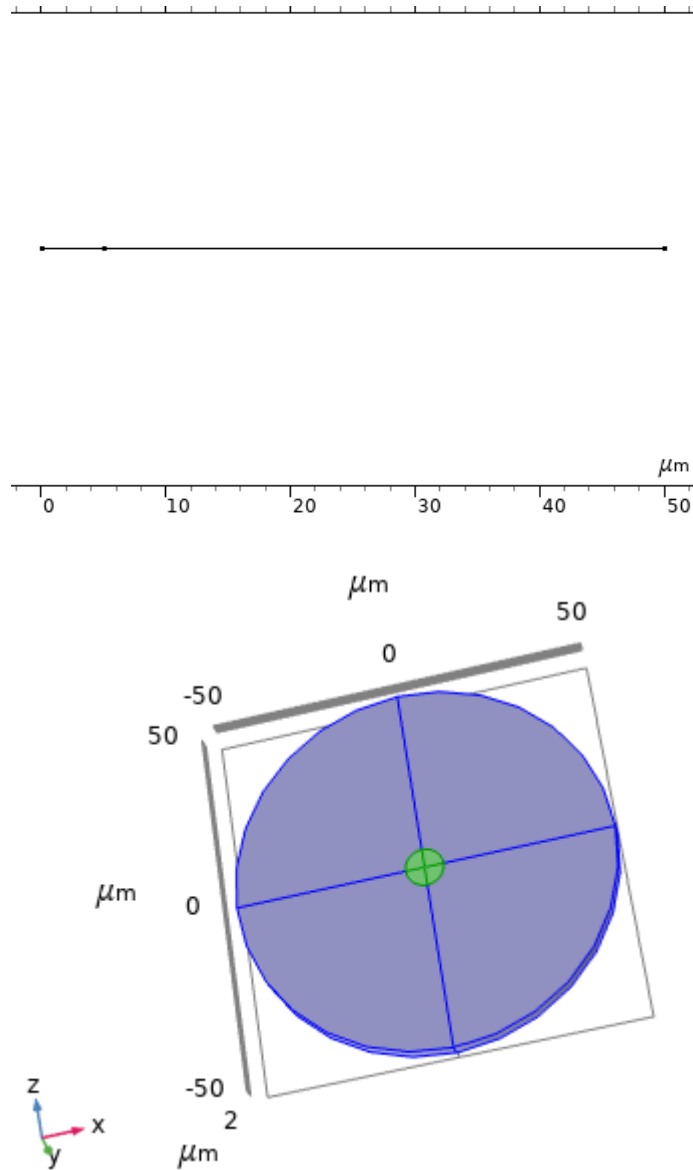
- TFM.mph (root)
- Global Definition
- Material
- Component
- Definition
- Reaction
- G-Values
 - Parametric Sweep
 - Step 1: Time Dependent
 - Solver Configurations
 - Job Configurations

The screenshot shows the 'Generate Space-Dependent Model' component settings panel. The panel is titled 'Generate Space-Dependent Model' and has a label 'Generate Space-Dependent Model 1'. The settings are organized into several sections:

- Space-Dependent Model Generation**: Contains a 'Create/Refresh' button.
- Component Settings**: Contains a 'Component to use:' dropdown menu set to '3D: New'.
- Physics Interfaces**: Contains several interface settings:
 - Chemical species transport: Transport of Diluted Species: New
 - Fluid flow: Darcy's Law: New
 - Heat transfer: Heat Transfer in Fluids: New
- Study Type**: Contains a 'Study type:' dropdown menu set to 'Time dependent'.

The left pane shows the component tree with 'Generate Space-Dependent Model' selected. Below it, the 'Equation View' is visible, showing a tree structure for 'G-Values' including 'Parametric Sweep', 'Step 1: Time Dependent', 'Solver Configurations', 'Job Configurations', 'Results', 'Datasets', 'Views', 'Derived Values', 'Tables', and 'Reports'.

Retos:



Model Builder

- Component 2 (comp2)
 - Definitions
 - Geometry 1(3D)
 - Materials
 - Chemistry 1 (chem)
 - Transport of Diluted Species (tds)
 - Transport Properties 1
 - No Flux 1
 - Initial Values 1
 - Reactions 1
 - Equation View
 - Heat Transfer in Fluids 1 (ht)
 - Fluid 1
 - Equation View
 - Initial Values 1
 - Thermal Insulation 1
 - Heat Source 1
 - Equation View
 - Darcy's Law 1 (dl)
 - Fluid and Matrix Properties 1
 - No Flow 1
 - Initial Values 1
 - Equation View
 - Mesh 1
 - G-Values
 - Study 2
 - Results

Settings

Transport of Diluted Species

Label: Transport of Diluted Species

Name: tds

Domain Selection

Selection: Manual

<input checked="" type="checkbox"/>	1
<input type="checkbox"/>	2

Equation

Equation form:

Study controlled

Show equation assuming:

Study 2, Time Dependent

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i$$

$$\mathbf{J}_i = -D_i \nabla c_i$$

Transport Mechanisms

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- [1] N.M. Schneider, M.M. Norton, B.J. Mendel, J.M. Grogan, F.M. Ross, H.H. Bau, Electron-Water interactions and implications for liquid cell electron microscopy, *J. Phys. Chem. C.* 118 (2014) 22373–22382. <https://doi.org/10.1021/jp507400n>.
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- [3] T. Gupta, N.M. Schneider, J.H. Park, D. Steingart, F.M. Ross, Spatially dependent dose rate in liquid cell transmission electron microscopy, *Nanoscale.* 10 (2018) 7702–7710. <https://doi.org/10.1039/c8nr01935e>.
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- [5] N.M. Schneider, Electron Beam Effects in Liquid Cell TEM and STEM 7.2 Electron Energy Loss in Liquids, (2017) 140–163.

Muchas gracias por su atención

