Matemáticas en Acción
Universidad de Cantabria, 17 de marzo de 2010.

Simulación Numérica de Procesos Industriales

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ÍNDICE

El informe de la OCDE (Julio 2008)

(Organisation for Economic Co-operation and Development)

http://www.oecd.org/dataoecd/47/1/41019441.pdf

Contents Executive Summary

5. Conclusions and Recommendations

- Industry faces problems that extend well beyond the envelope of classical topics in mathematics.
- Many of these problems have a significant mathematical component, and the intellectual challenges they pose fall in many cases within topical areas of current research in the mathematical sciences.
- Stronger links between mathematics and industry will be beneficial both to the partners and to national economies.
- They will inspire new mathematics and enhance the competitive advantage of companies.

- Several countries have developed a variety of mechanisms to facilitate a constructive relationship between mathematics and industry; in these countries, dynamic collaborations already exist.
- In others, there is an urgent need to create or revitalize the connection. Governments can play a role, notably through national funding agencies.
- This section of the report contains recommendations that can improve the interface.
- They have been suggested by the workshop participants and are addressed to the academic community, governmental and other funding agencies, and industry.
- The list reflects best practices and is meant to be indicative; it is by no means exhaustive, and not all recommendations may apply in particular situations.

5.1 Mathematics for Industrial Innovation

5.2 Education and Training

5.3 The Interface between Mathematics and Industry

5.4 Academic Infrastructure

5.5 Industrial Infrastructure

5.6. National and International Coordination

5.7 Action Items

Forward Look on Mathematics and Industry (ESF)

Proposal for
a Forward Look on
Mathematics and Industry

Presented by

Professor Mario Primicerio,

on behalf of

The Applied Mathematics Committee of the European Mathematical Society

to

The European Science Foundation

Objectives

- Mathematics provides a universal framework for innovation, which is vital for society and industry.
- However, the interaction between mathematics and industry is far from optimal.
- Consequently, a strong inter-connected community and a vision for Europe are needed more than ever.

- This Forward Look[a] is aimed at analysing the current state of interaction between mathematics and Industry.
- Through its analyses and recommendations, it will enable the scientific and industrial communities, together with policy makers, to develop medium to long-term strategies for future research activities and applications.
- It is expected that it will impact society by strengthening the mathematical knowledge base of a wide spectrum of research-intensive industries.
- One key goal is thus to define well-adapted and ambitious research and political agendas at national and European levels.

[a] Initiated by the Centre National de la Recherche Scientifique (CNRS) in France and developed with the support of the Physical and Engineering Sciences (PESC) Unit and the Chief Executive Unit of ESF.

Work-plan

- The Forward Look will build on the results of the report on "mathematics and industry" from the Organisation for Economic Co-operation and Development (OECD) by focussing on the specificities of the European context such as its strength, its fragmentation and diversity.
- It will directly involve Academia and Industry as well as policy-makers.
- It will systematically include past extensive experiences in the cooperation between academic and industrial researchers together with the political views.

- Three working groups will concentrate on specific topics, “Training and career development”, “Academia-Industry interface” and “Opportunities and challenges”.
- After the initial launch of the Forward Look, thematic foresight activities are planned to take place over one year.
- The results will be presented in a joint draft report in a consensus conference.
- Eventually, after incorporating feedback from the relevant communities, the final document will be released in a publicised closing event and disseminated widely.

Forward Look Mathematics and Industry. Consensus Conference

Madrid, 26 y 27 de abril de 2010.

http://www.ceremade.dauphine.fr/FLMI/Consensus_Conference_Madrid/index.html

Matemáticas para la industria en Europa: el informe MACSI-net (2004)

Red europea: Matemathics, Computing and Simulation for Industry

1. Technische Universiteit Eindhoven,Netherlands
2. Johannes Keppler Universität Linz, Austria
3. Vrije Universiteit Brussel, Belgium
4. Denmarks Tekniske Universitet, Lyngby, Denmark
5. Jyväskylän Yliopisto / University of Jyväskylän, Finland
6. Dassault Aviation, France
7. Institut National de Recherche en Informatique et Automatiques, Sophia Antipolis, France
8. Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern, Germany
9. Konrad-Zuse-Zentrum für Informationstechnik Berlin, Germany
10. National Technical Unversity Athens, Greece
11. Università degli Studi di Milano, Italy
12. Università degli Studi di Padova, Italy
13. Norges Teknisk-Naturviten-skapelige Universitet, Trondheim, Norway
14. International Center for Numerical Methods in Engineering, Barcelona, Spain

15. Universidade de Santiago de Compostela, Spain
16. Chalmers University of Technology, Gothenburg, Sweden
17. Ecole Polytechnique Fédérale de Lausanne, Switzerland
18. Seminar for Applied Mathematics, Eidgenössische Technische Hochschule Zürich, Switzerland
19. OCIAM, University of Oxford, United Kingdom University of Wales at Swansea, United Kingdom
20. University of Innsbruck, Austria
21. University of Bayreuth, Germany
22. International Centre for Mechanical Sciences, Udine, Italy
23. Weierstrass-Institut für Angewandte Analysis und Stochastik im Forschungsverbund, Berlin, Germany

MATHEMATICS: Key for the European Knowledge-based Economy. A Roadmap for Mathematics in European Industry,
(http://www.macsinet.org/newsletter.htm)

TEMAS:

'...six technology themes clearly emerge as being of central importance in industry':

- simulation of processes and products,
- optimization, control and design,
- uncertainty and risk,
- management and exploitation of data,
- virtual material design,
- biotechnology, food and health.

Estos temas están relacionados al menos con las siguientes áreas de las matemáticas:

- Modelización matemática
- Ecuaciones en derivadas parciales
- Análisis numerico
- Teoría de optimización y control
- Investigación operativa
- Matemática discreta
- Probabilidad
- Estadística

MATHEMATICAL MODELLING, NUMERICAL SIMULATION AND COMPUTATIONAL SCIENCE

Computational Science

Computational Science and Engineering (CSE)

Do not confuse with Computer Science (Informática)

De WIKIPEDIA

- Ciencia Computacional (o Cálculo Científico) es el campo de estudio que trata de la construcción de modelos matemáticos y de técnicas numéricas de resolución, así como del uso de los computadores, para analizar y resolver problemas de la ciencia, de las ciencias sociales y de la ingeniería.

- Este campo es distinto de la "computer science" (informática) (el estudio matemático de la computación, los ordenadores y el procesado de la información).

- Científicos e ingenieros desarrollan programas de ordenador, software de aplicación que modeliza los sistemas objeto de estudio y ejecutan esos programas con varios conjuntos de parámetros de entrada.

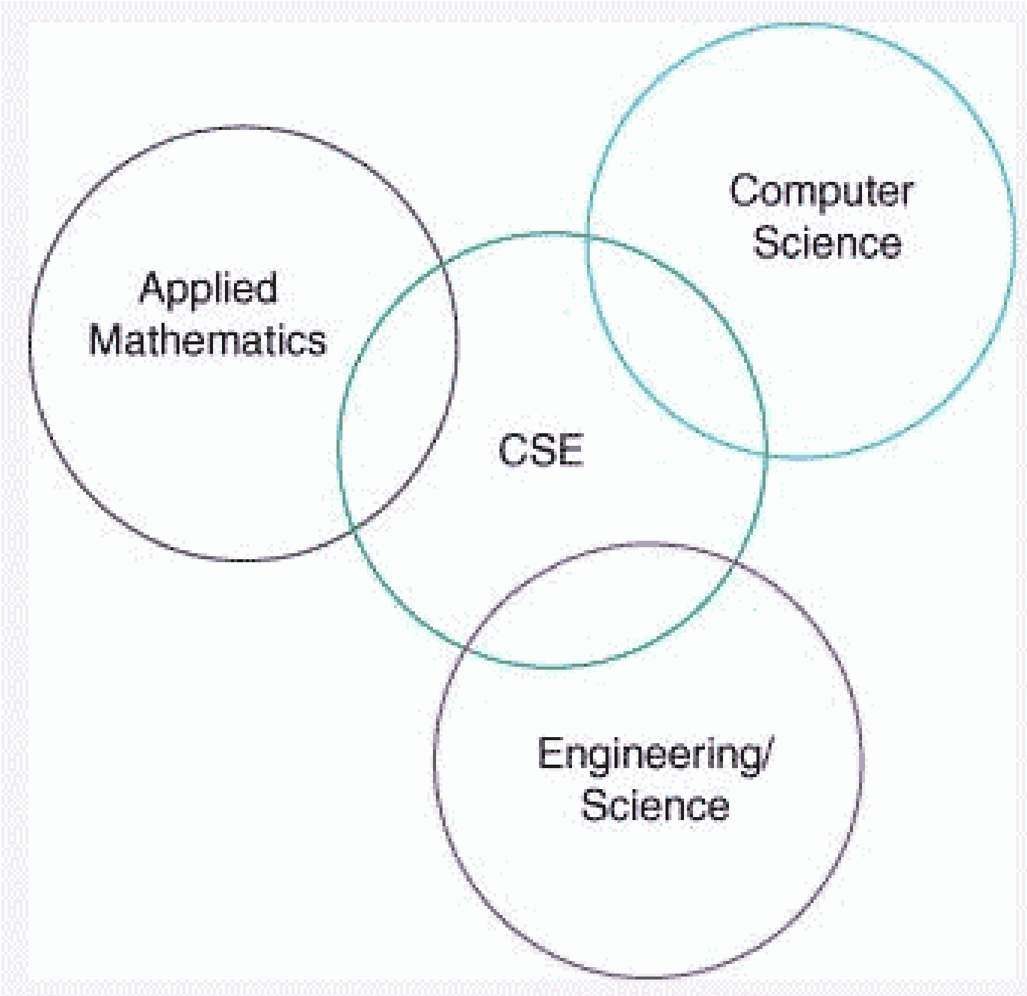
- Típicamente esos modelos requieren cantidades enormes de cálculos (generalmente en punto flotante) y son a menudo ejecutados en supercomputadores o en plataformas de cálculo distribuido.

La Ciencia computacional está relacionada (al menos) con las siguientes áreas de la matemáticas

- Modelización matemática
- Ecuaciones en derivadas parciales
- Análisis numérico

- Ejemplos de áreas de aplicación son
  - la mecánica de fluidos (aerodinámica de automóviles y aviones, procesos de combustión, dispersión de la contaminación,...),
  - diseño de materiales
  - tecnología de semiconductores (crecimiento de cristales, procesos de oxidación),
  - predicción del tiempo y del clima (formación de tornados, calentamiento global),
  - matémática financiera (gestión de carteras, cálculo del precio de productos derivados,...).

- La Ciencia Computacional se ha convertido en el tercer pilar del método científico, al lado de la teoría y la experimentación.


Applied Mathematics
Computer Science
CSE
Engineering/ Science

Metodología

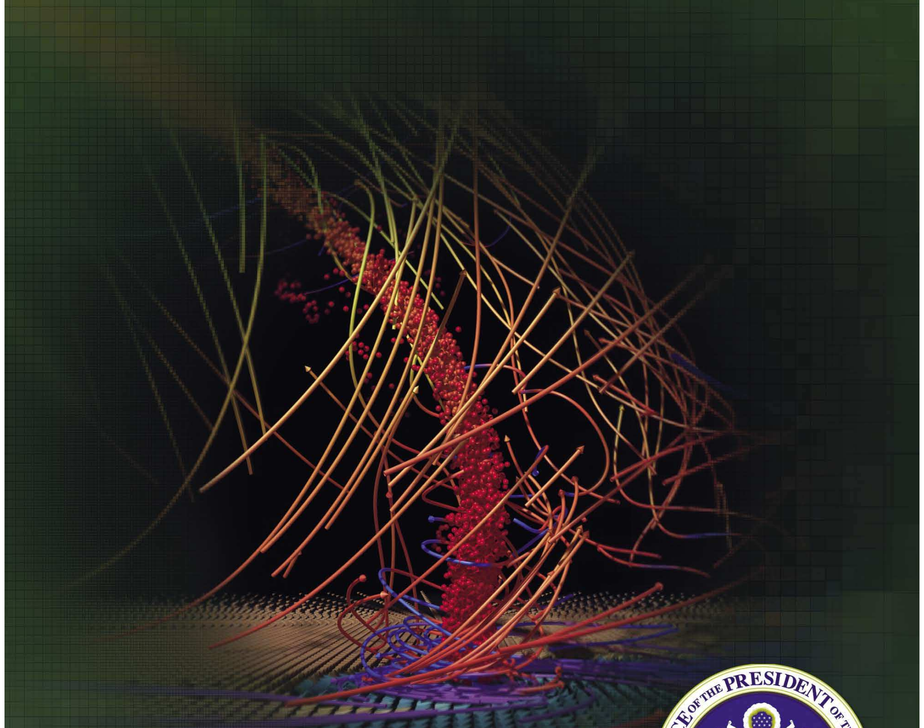
Básicamente, se pueden distinguir varias etapas en el proceso de simulación:

1. Establecimiento de un modelo.
2. Análisis matemático.
3. Análisis numérico.
4. Implementación en ordenador.
5. Empaquetamiento.
6. Visualización
7. Validación.

REPORT TO THE PRESIDENT

JUNE 2005

COMPUTATIONAL SCIENCE: ENSURING AMERICA'S COMPETITIVENESS



PRESIDENT'S
INFORMATION TECHNOLOGY
ADVISORY COMMITTEE

EXECUTIVE OFFICE OF THE PRESIDENT OF THE UNITED STATES
PRESIDENT'S INFORMATION TECHNOLOGY ADVISORY COMMITTEE

Principal Finding

- Computational science is now indispensable to the solution of complex problems in every sector, from traditional science and engineering domains to such key areas as national security, public health, and economic innovation.
- Advances in computing and connectivity make it possible to develop computational models and capture and analyze unprecedented amounts of experimental and observational data to address problems previously deemed intractable or beyond imagination.

- Yet despite the great opportunities and needs, universities and the Federal government have not effectively recognized the strategic significance of computational science in either their organizational structures or their research and educational planning.
- These inadequacies compromise U.S. scientific leadership, economic competitiveness, and national security.

Principal Recommendation

- Universities and the Federal government's R&D agencies must make coordinated, fundamental, structural changes that affirm the integral role of computational science in addressing the 21st century's most important problems, which are predominantly multidisciplinary, multi-agency, multisector, and collaborative.
- To initiate the required transformation, the Federal government, in partnership with academia and industry, must also create and execute a multi-decade roadmap directing coordinated advances in computational science and its applications in science and engineering disciplines.

Iniciativas en España: el proyecto Consolider i-MATH

- Ingenio MATHEMATICA (i-MATH) is a CONSOLIDER singular research project for the period 2006-2011.
- It proposes a complete activity research program for Spanish mathematics, with the purpose of promoting and carrying out strategic actions of national scope that qualitatively and quantitatively increase mathematical presence on the international scene, and in the Spanish system of science, technology and business and on the international scene.

- i-MATH is an initiative promoted and financed by the Spanish Ministry of Education and Science with a budget of 7,500,000 euros (5 years).
- i-MATH is a network structured around
  - a coordinator-researcher (Marco A. López Cerdá),
  - a management center (University of Cantabria),
  - a steering commitee (SC),
  - five nodes (CESGA, CIEM, CRM, ICMAT and IMUB)
  - and more than 300 principal researchers (PRs) and their research groups.

The Research Activity Program of i-MATH covers a very wide scope and is structured around four main thematic areas:

- From basic research to applications
- How to understand the physical world
- The essential computational support
- Direct applications to society

The official start of the i-MATH project was the 3rd of October, 2006.

Aplicaciones de la simulación numérica en la industria. Ejemplos

Silicio: producción y aplicaciones

- El silicio **se produce** en **hornos de arco eléctrico** por reducción del **dióxido de silcio** con **carbono**:

$$\mathrm{Si\,O_2} + \mathrm{C} = \mathrm{Si} + \mathrm{C\,O_2}$$

Silicio: producción y aplicaciones

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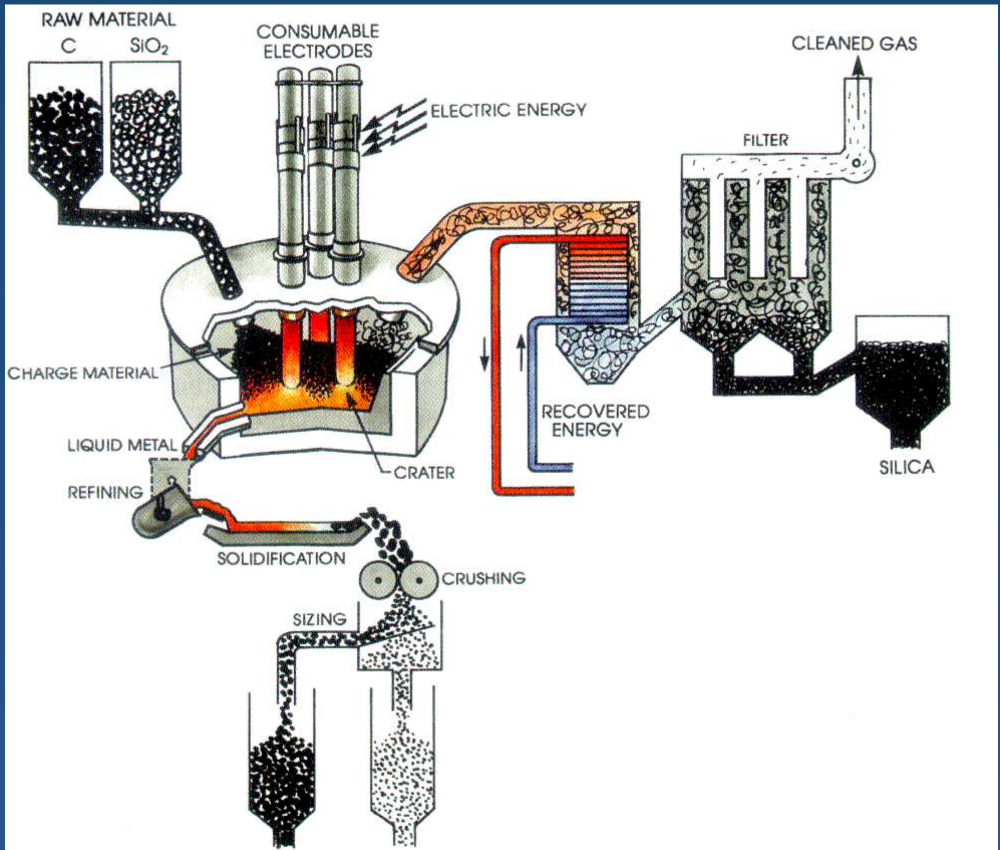
$$\mathrm{Si\ O_2 + C = Si + C\ O_2}$$



Silicio: producción y aplicaciones

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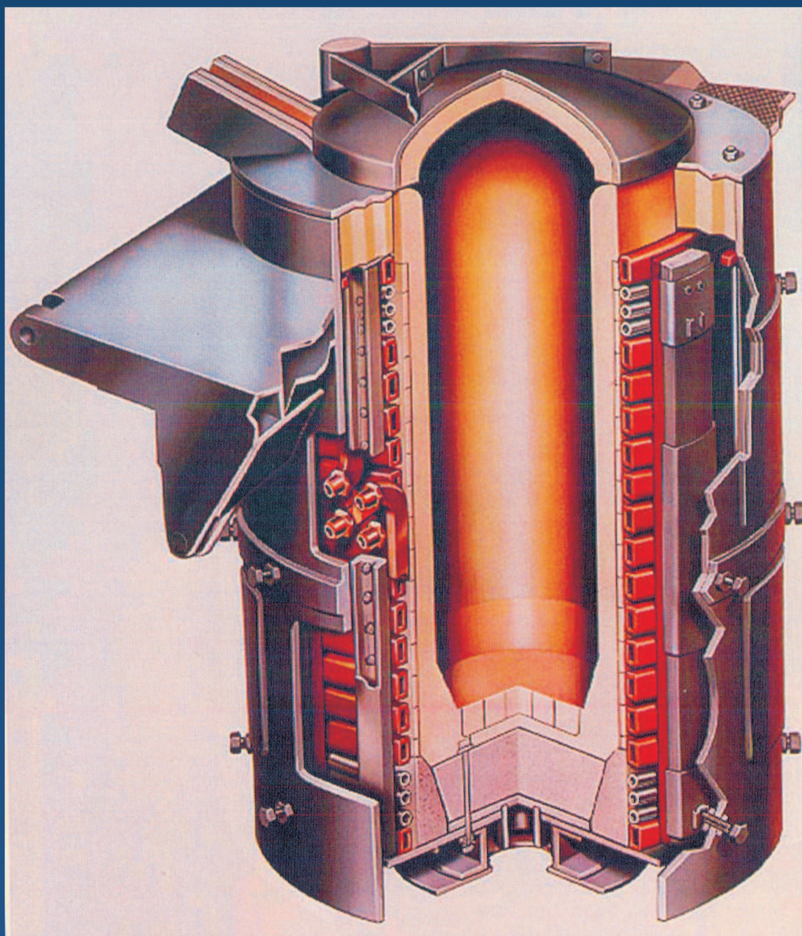
Aplicaciones:

- Ferrosilicio (aceros al silicio, puede contener mas de un 2% de otros materiales)
- Silcio metalúrgico (e.g. aleaciones alumnio-silicio, contiene en torno a 1% de otrso elementos)
- Silcio químico (siliconas)
- Silicio solar (células fotovoltaicas)
- Silicio electrónico (semiconductores, el silicio más puro, "9N" = 99.9999999 de pureza)

El problema físico

Fotografías tomadas de http://www.ameritherm.com

Un horno de inducción industrial



- Silicio para fundir y purificar
- Crisol de grafito
- Capas refractarias
- Bobina refrigerada con agua

Modelo matemático

Problemas acoplados

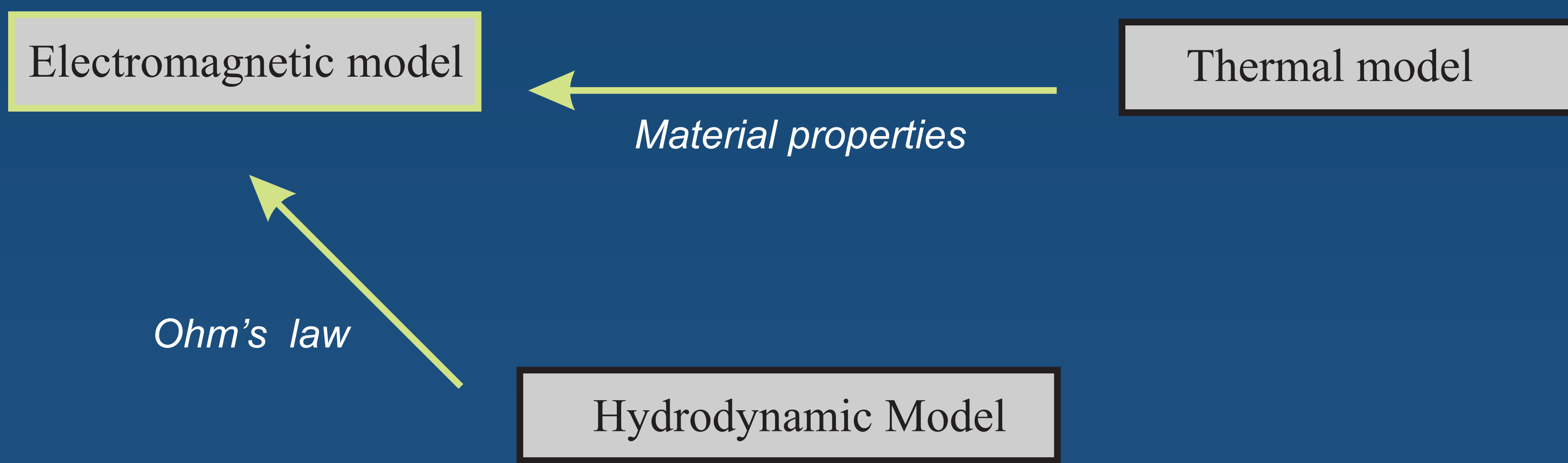
Electromagnetic model

Thermal model

Hydrodynamic Model

Modelo matemático

Modelo electromagnético

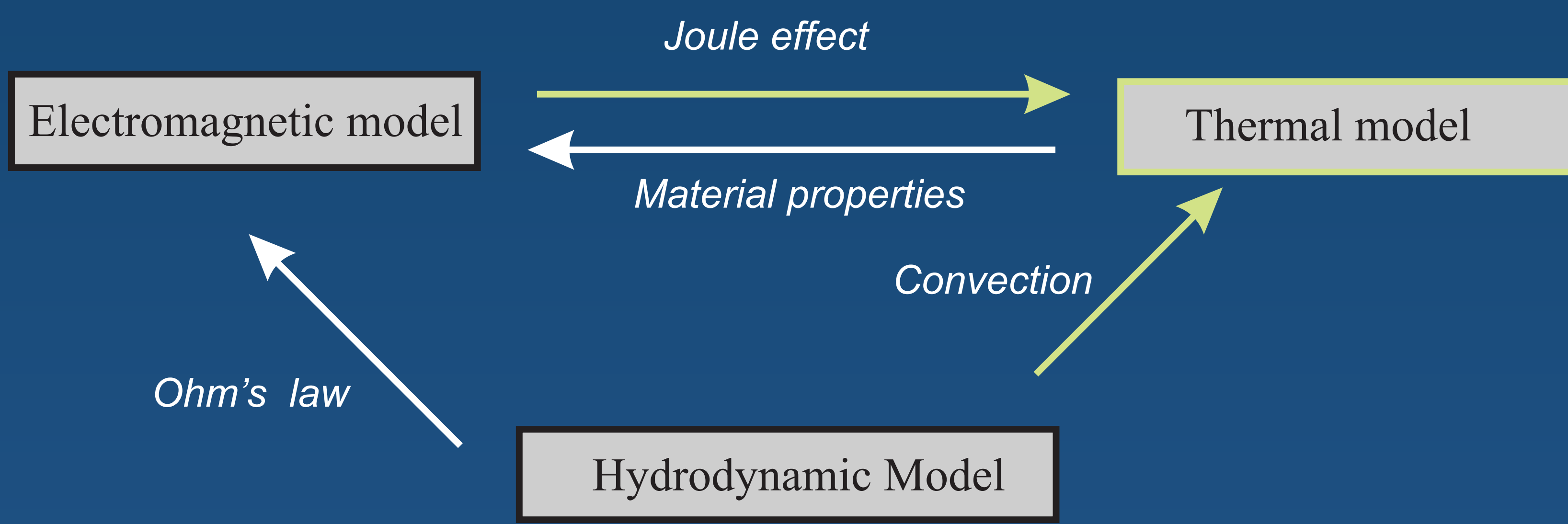


$$\begin{aligned} \mathbf{curl}\,\mathbf{H} &= \mathbf{J}, \\ i\omega\mathbf{B} + \mathbf{curl}\,\mathbf{E} &= \mathbf{0}, \\ \mathrm{div}\,\mathbf{B} &= 0, \end{aligned}$$

$$\begin{aligned} \mathbf{B} &= \mu(T)\mathbf{H}, \\ \mathbf{J} &= \sigma(T)(\mathbf{E} + \mathbf{v} \times \mathbf{B}). \end{aligned}$$

Modelo matemático

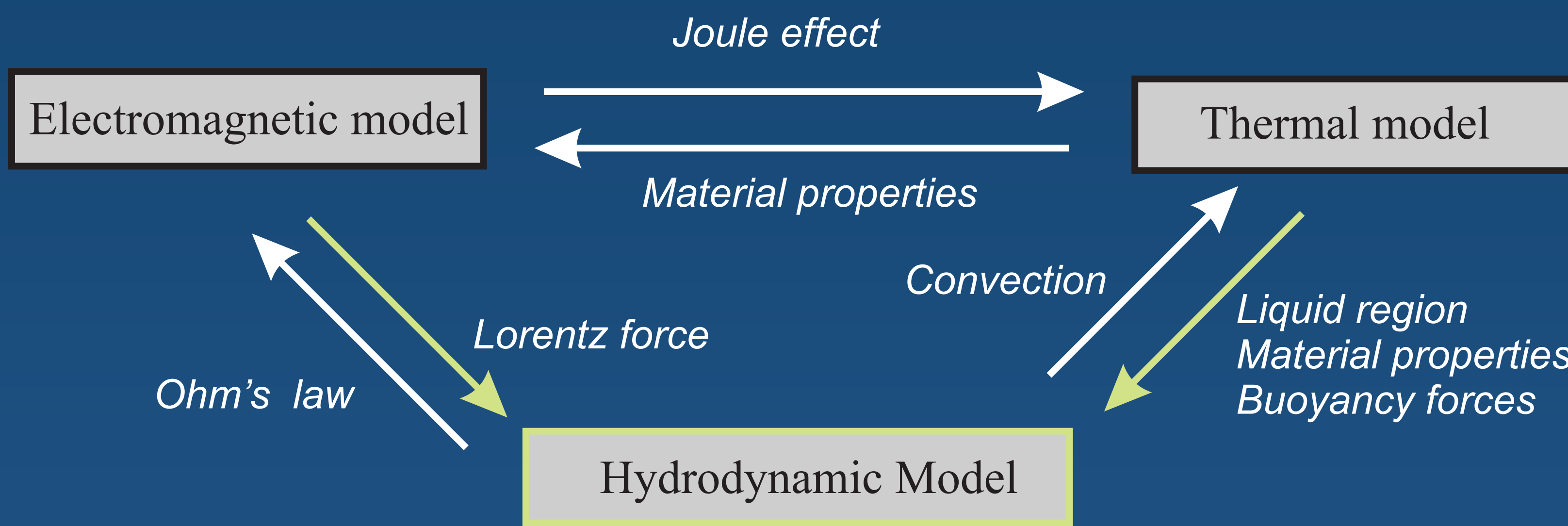
Modelo térmico



$$\frac{\partial e}{\partial t} + \mathbf{v} \cdot \mathbf{grad}\, e - \mathrm{div}\,(k\, \mathbf{grad}\, T) = \frac{|\mathbf{J}|^2}{2\sigma}$$

Modelo matemático

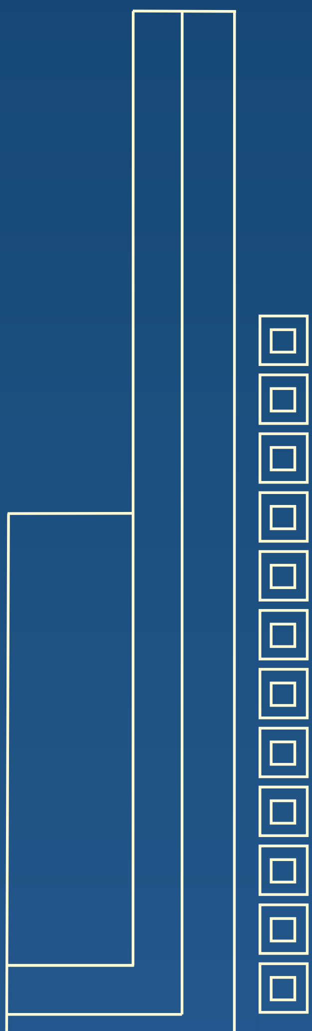
Modelo hidrodinámico



$$\begin{aligned} \rho(T)\dot{\mathbf{v}} - \operatorname{div}\left(\eta(T)(\operatorname{grad}\mathbf{v} + (\operatorname{grad}\mathbf{v})^t)\right) + \mathbf{grad}\, p &= \mathbf{f}(T,\mathbf{H}) \\ \operatorname{div}\mathbf{v} &= 0 \end{aligned}$$

Resultados numéricos: un horno indistrial

Silicio dentro de un crisol de grafito y una capa de material refractario



Datos geométricos

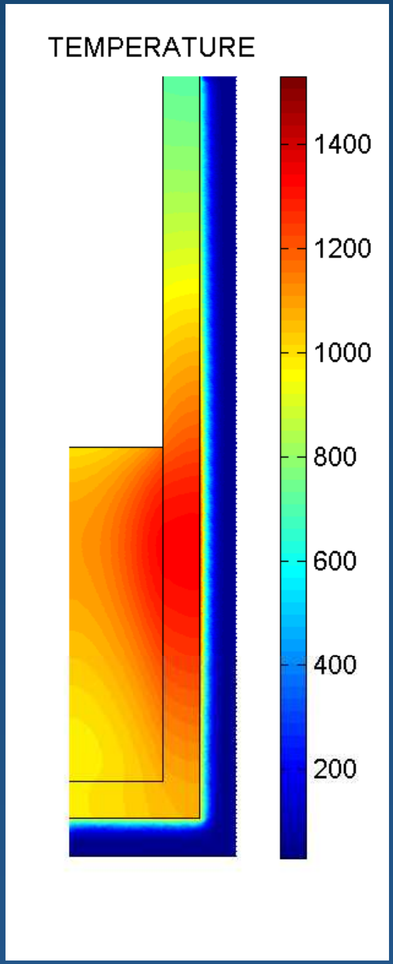
Altura del silicio:	0.45 m
Radio interior del crisol:	0.125 m
Radio exterior del crisol:	0.225 m
Altura del crisol:	1.05 m
Diámetro de la bobina:	0.05 m
Distancia de la bobina al refractario:	0.025 m
Distancia entre espiras:	0.01 m
Número de espiras :	12

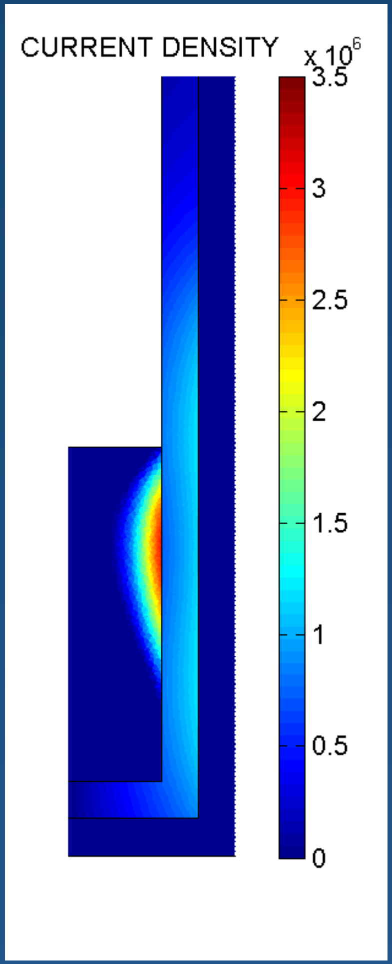
Parámetros de trabajo

Frecuencia:	100 Hz
Intensidad de corriente:	5500 A

Resultados numéricos: f=100 Hz, I=5500 A

Temperatura y densidad de corriente

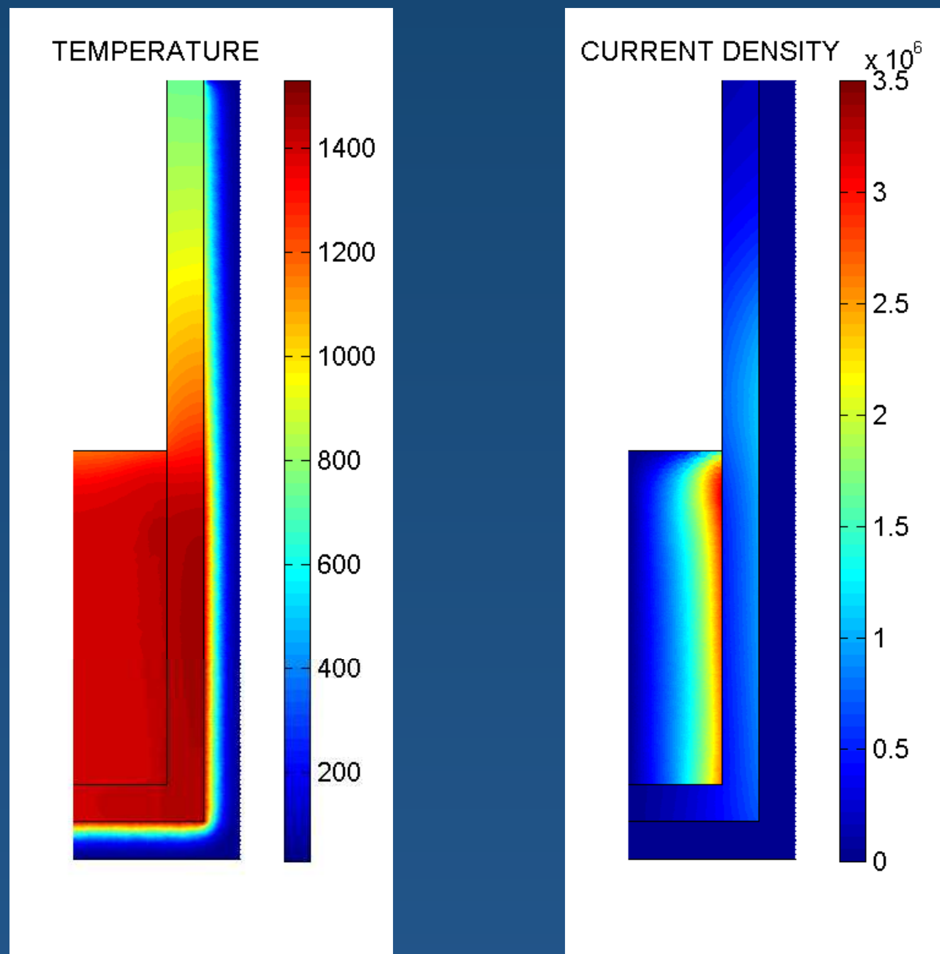




$$t = 30\ min$$

Resultados numéricos: f=100 Hz, I=5500 A

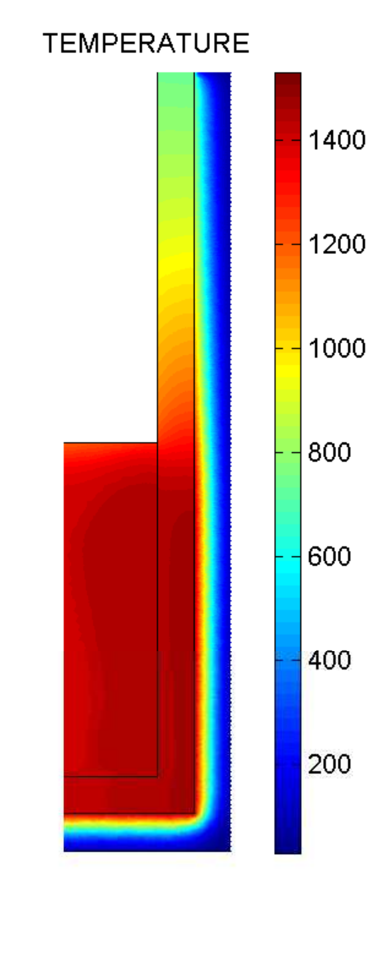
Temperatura y densidad de corriente

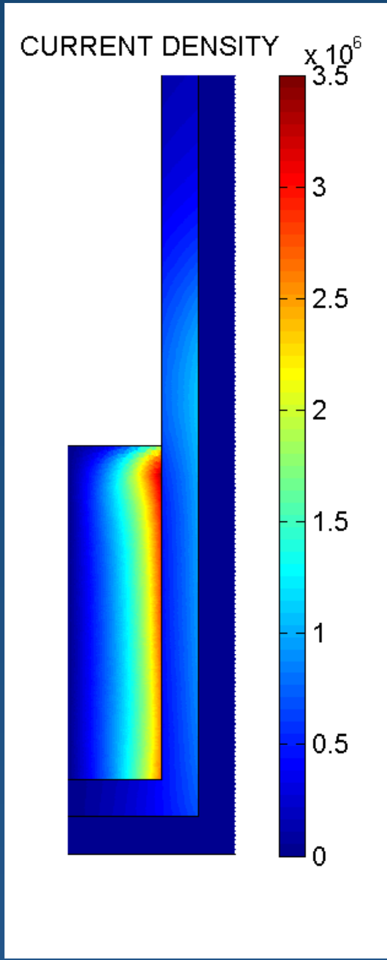


$$t = 60\ min$$

Resultados numéricos: f=100 Hz, I=5500 A

Temperatura y densidad de corriente

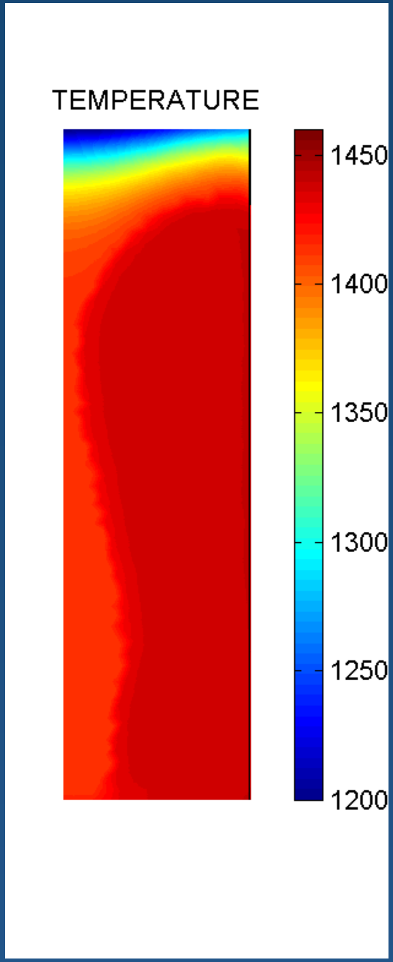


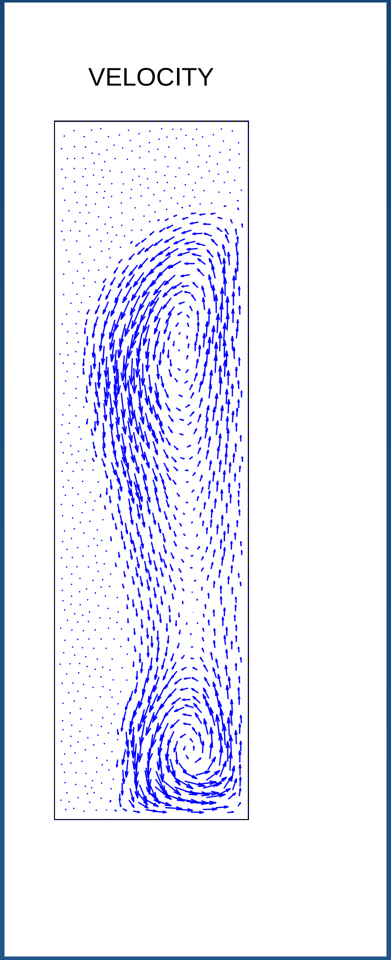


$$t = 90\ min$$

Resultados numéricos: f=100 Hz, I=5500 A

Temperatura y velocidad en el silicio

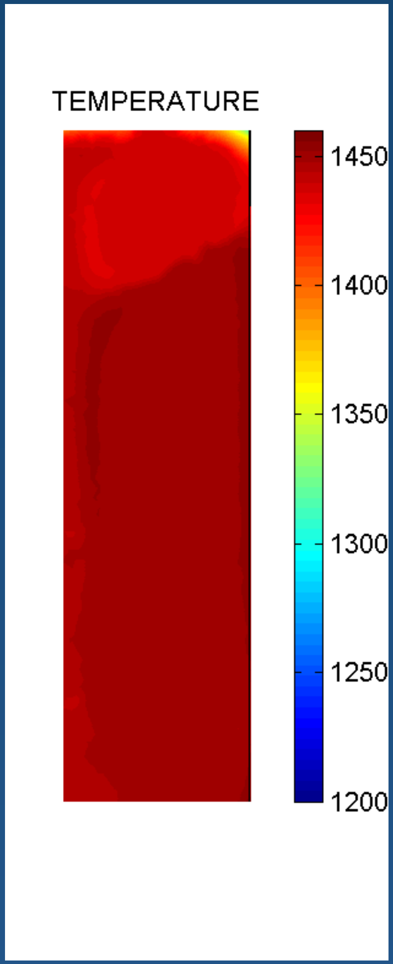


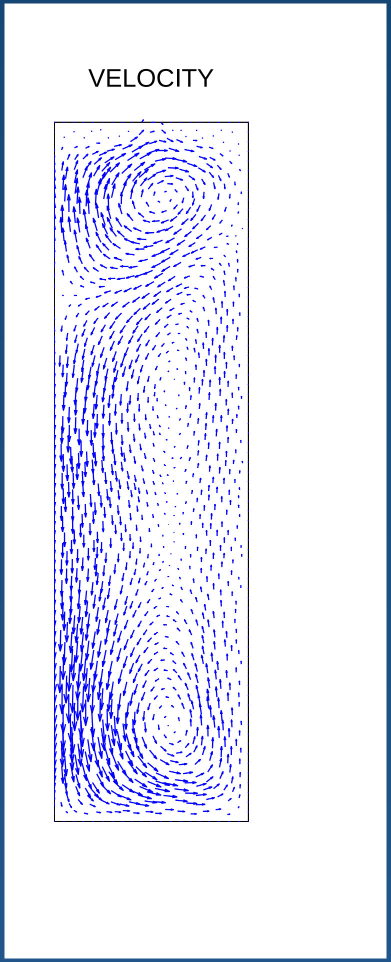


$$t = 90\ min$$

Resultados numéricos: f=100 Hz, I=5500 A

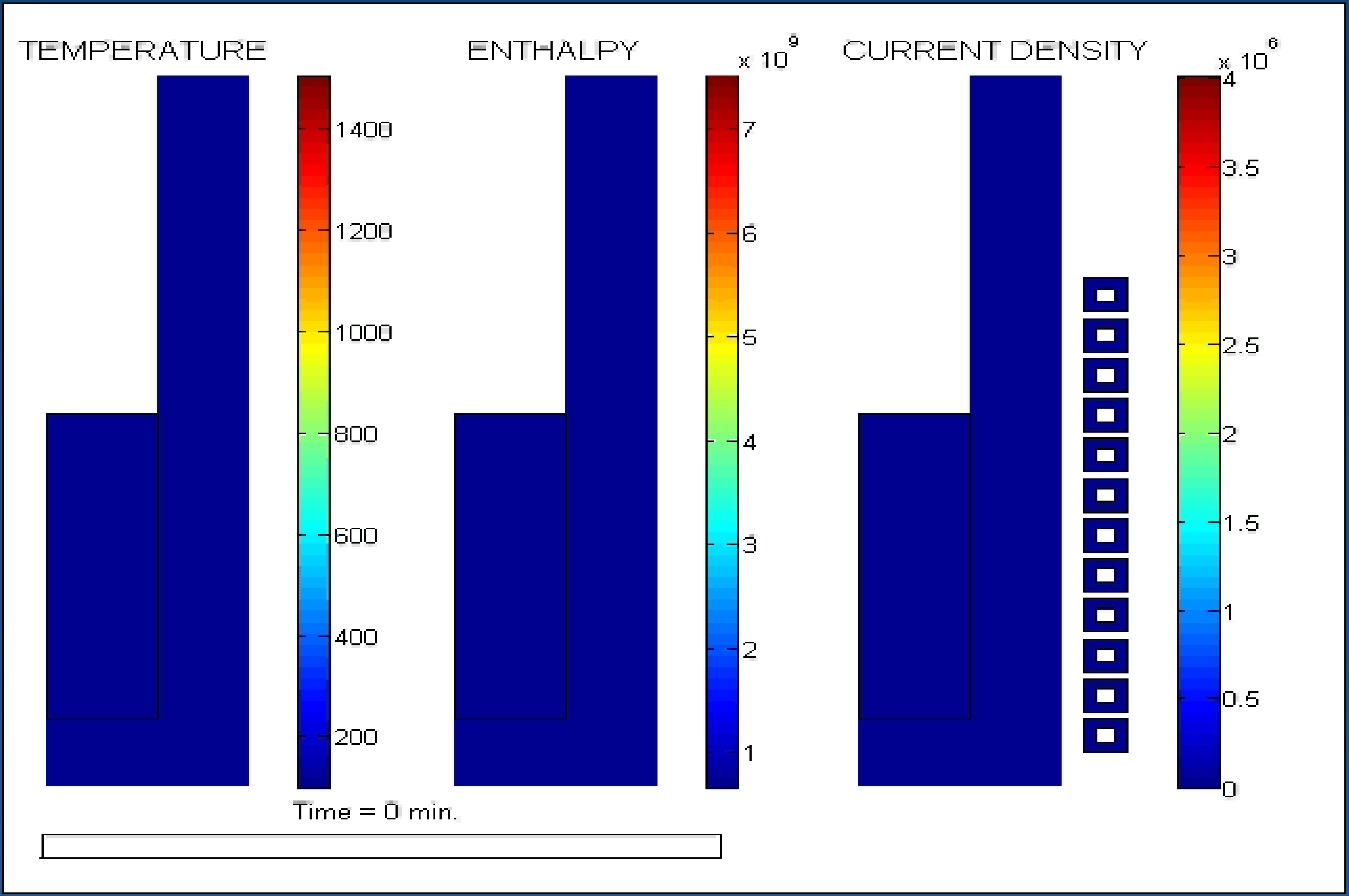
Temperatura y densidad de corriente



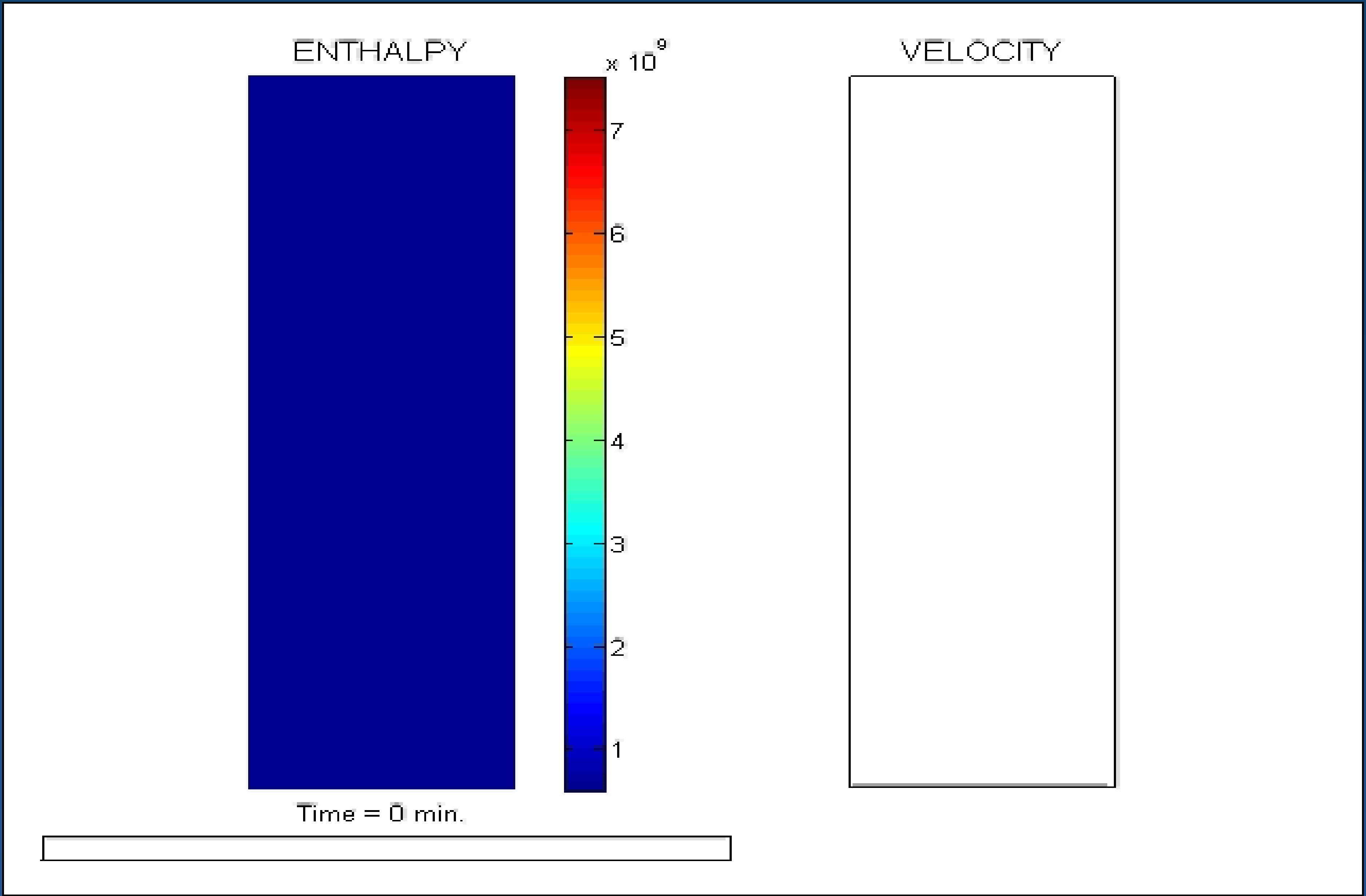


$$t = 180\ min$$

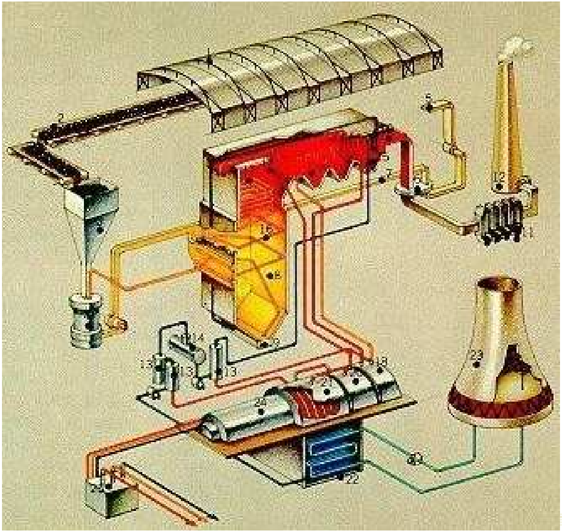
Evolución de la temperatura, la entalpía y la densidad de corriente.



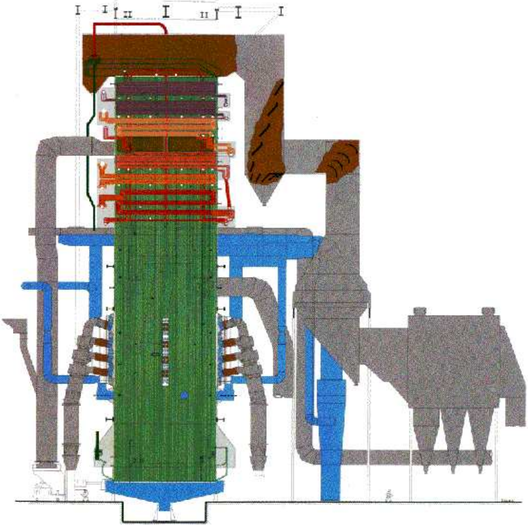
Evolución de la entalpía y la velocidad en el silicio.



Sketch of a power plant



Coal-fired boiler



Mathematical modeling of coal-fired boilers

Main features

- Two-phase flow
- Homogeneous and heterogeneous chemical reactions of combustion
- Compressible turbulent flow
- Radiative heat transfer
- Geometric complexity. Large number of inlets (burners).

Mathematical modeling of coal-fired boilers

Model for the gas phase

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = f^m,$$

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \otimes \vec{v}) + \nabla p = \nabla \cdot (l(D)) + \vec{b} + \vec{f}_q,$$

$$\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho h \vec{v}) - \nabla \cdot (\rho \mathcal{D} \nabla h) - \dot{p} + \nabla \cdot \vec{q}_r = l(D) \cdot D + f^h,$$

$$\frac{\partial y_i}{\partial t} + \nabla \cdot (y_i \vec{v}) - \nabla \cdot (\mathcal{D}\, \nabla y_i) = w_i + f_i^m, \ i = 1, \ldots, N,$$

$$\omega \cdot \nabla_x I = -aI + aI_b - \sigma_s I + \frac{\sigma_s}{4\pi} \int_{S^2} \phi(\omega^*, \omega) I(\omega^*) d\omega^*.$$

Mathematical modeling of coal-fired boilers

Model for the gas phase

$$
\begin{aligned}
p &= \rho R \theta, \\
R &= \frac{\mathcal{R}}{\mathcal{M}} = \mathcal{R} \sum_{i=1}^{N} \frac{Y_i}{\mathcal{M}_i}, \quad (Y_i = \frac{1}{\rho} y_i \mathcal{M}_i, \text{ mass fraction}), \\
l(D) &= 2\eta D + \xi \nabla \cdot \vec{v} I, \quad D = \frac{1}{2}(\nabla \vec{v} + \nabla \vec{v}^t) \\
h &= \sum_{i=1}^{N} Y_i [\hat{h}_i(\theta_0) + \int_{\theta_0}^{\theta} \hat{c}_{\pi,i}(s)\, ds], \\
w_i &= \sum_{l=1}^{L} (\lambda_i^l - \nu_i^l) \delta_l, \; i = 1, \ldots, N, \\
\delta_l &= k_l \prod_{j=1}^{N} y_j^{\nu_j^l}, \; l = 1, \cdots, L \\
k_l(\theta) &= B_l \theta^{\alpha_l} e^{-\frac{\mathcal{E}_l}{\mathcal{R}\theta}}.
\end{aligned}
$$

Mathematical modeling of coal-fired boilers

Numerical solution is very difficult

Mathematical modeling of coal-fired boilers

Numerical solution is very difficult

- Coupled system of non-linear partial differential equations.

Mathematical modeling of coal-fired boilers

Numerical solution is very difficult

- Coupled system of non-linear partial differential equations.
- Nonlinear **stiff** source terms modeling gas-phase chemical reactions.

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- Coupled system of non-linear partial differential equations.
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The problem is much simpler

- either assuming **local chemical equilibrium**

Mathematical modeling of coal-fired boilers

Numerical solution is very difficult

- Coupled system of non-linear partial differential equations.
- Nonlinear **stiff** source terms modeling gas-phase chemical reactions.

The problem is much simpler

- either assuming **local chemical equilibrium**
- or applying **high activation energy asymptotics** (*mixed is burnt*) leading to **diffusion flames**.

Mathematical modeling of coal-fired boilers

1. Local chemical equilibrium

Mathematical modeling of coal-fired boilers

1. Local chemical equilibrium

- FLUENT **mixture fraction/pdf** model for homogenous turbulent combustion in the gas phase

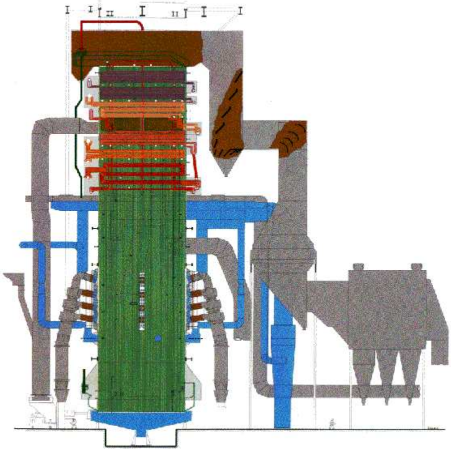
Mathematical modeling of coal-fired boilers

1. Local chemical equilibrium

- FLUENT **mixture fraction/pdf** model for homogenous turbulent combustion in the gas phase
- FLUENT Lagrangian **discrete phase** model for heterogeneous combustion of the coal particles

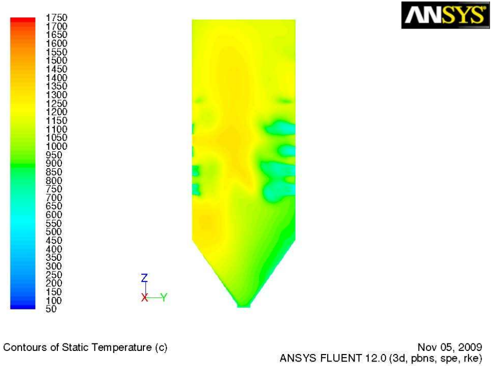
An example: ENDESA As Pontes power plant

Mathematical modeling of coal-fired boilers

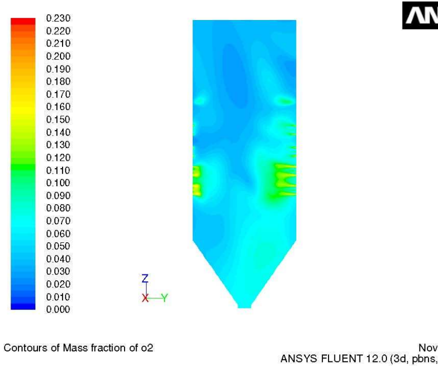


Numerical results

Temperature (vertical cut)

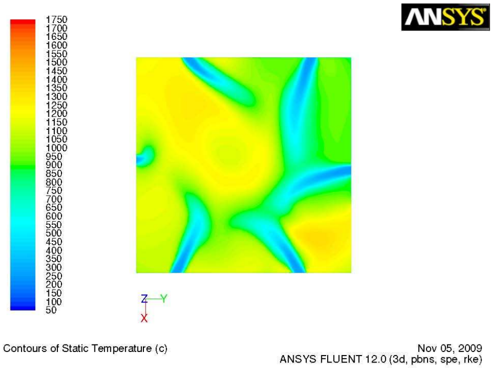


Oxygen

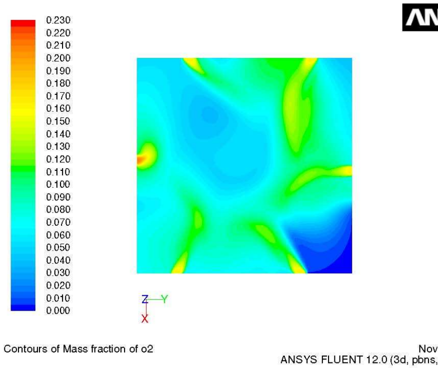


Numerical results

Temperature (horizontal cut)

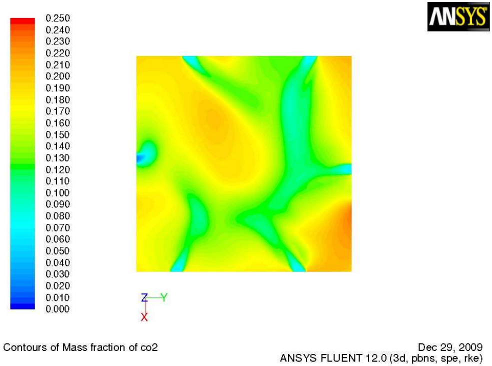


Oxygen

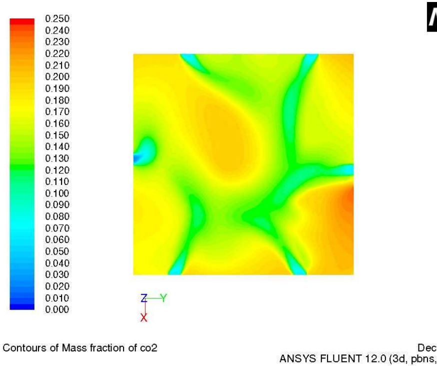


Numerical results

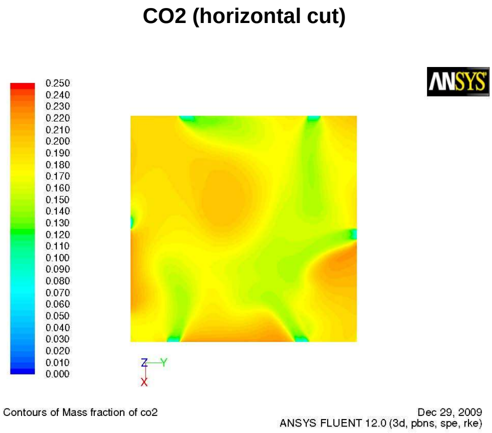
Carbon dioxide (horizontal cut)

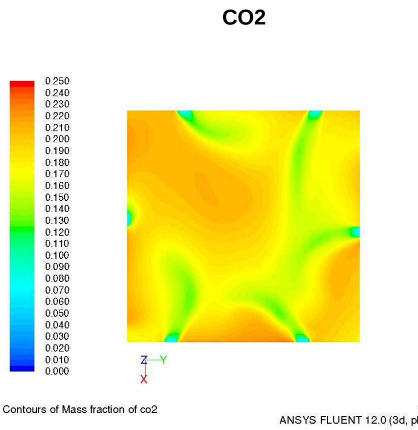


Carbon dioxide



Numerical results





A geochemical example: Introduction

Some hints of the project between the *Department of Applied Mathematics of the University of Santiago de Compostela* and the company *Lignitos de Meirama S.A.*, financed by the I+D+I Galician Government plan (2006-2010)

- Prediction of the water quality of a future pit lake in NW Spain.
- The lake, when filled, will be connected to a water reservoir. It has to satisfy certain water quality standards.
- Will these legal limits be fulfilled?

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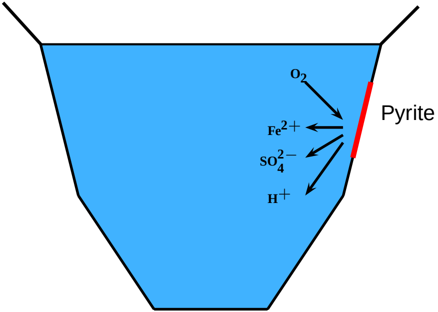
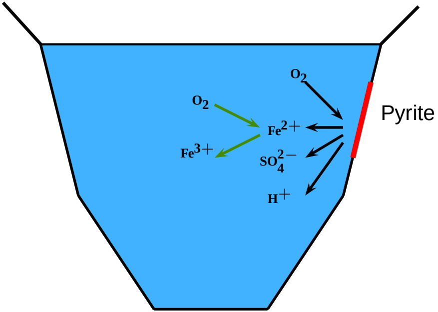
- Prediction of the water quality of a future pit lake in NW Spain.
- The lake, when filled, will be connected to a water reservoir. It has to satisfy certain water quality standards.
- Will these legal limits be fulfilled?
  We have to take into account
  - **The chemical composition of the wall rocks**
  - The magnitude and geochemistry of the water sources that flow into the pit.
  - The precipitation/evaporation ratio
  - The lake limnology
  - The biological activity...

A geochemical example: pyrite oxidation by O_2



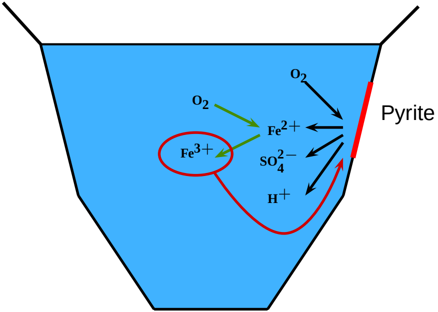
$$FeS_{2(s)} + 7/2O_{2(aq)} + H_2O \longrightarrow Fe^{2+}_{(aq)} + 2SO^{2-}_{4(aq)} + 2H^{+}_{(aq)}$$

A geochemical example: abiotic oxidation of Fe^{2+}



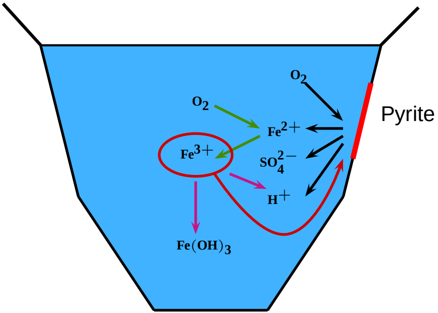
$$Fe^{2+}_{(aq)} + 1/4O_{2(aq)} + H^{+}_{(aq)} \longrightarrow Fe^{3+}_{(aq)} + 1/2H_2O_{(ac)}$$

A geochemical example: pyrite oxidation by Fe^{3+}



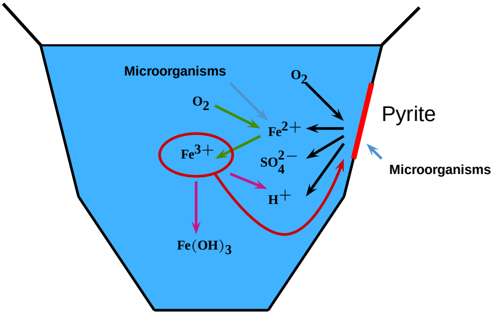
$$FeS_{2(s)} + 14Fe^{3+}_{(aq)} + 8H_2O \longrightarrow 15Fe^{2+}_{(aq)} + 2SO^{2-}_{4(aq)} + 16H^{+}_{(aq)}$$

A geochemical example: Ferrihydrite precipitation



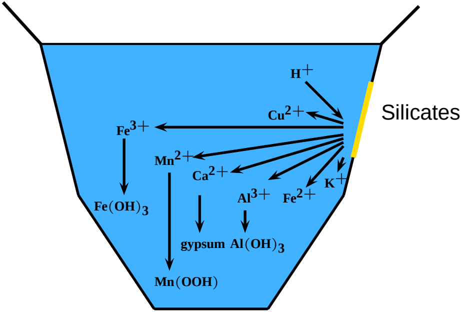
$$Fe^{3+}_{(aq)} + 3H_2O \longleftrightarrow Fe(OH)_{3(s)} + 3H^+_{(aq)}$$

A geochemical example: Ferrihydrite precipitation



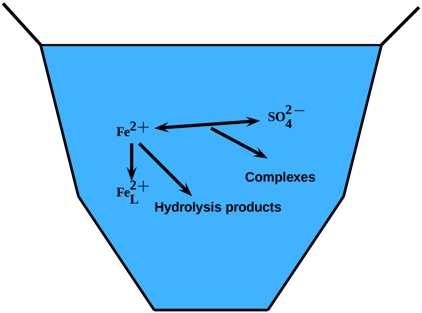
$$Fe^{3+}_{(aq)} + 3H_2O \longleftrightarrow Fe(OH)_{3(s)} + 3H^{+}_{(aq)}$$

A geochemical example: Silicate degradation



$$Silicates + H^+ \longrightarrow Heavy \quad metals$$

A geochemical example: Equilibrium reactions



A geochemical example: problem setting

The lake is assumed to be a stirred tank

The problem is stated by considering

- The chemical reactions before and much more... ▸ Show reactions
- The entrance of different water sources. ▸ Show sources
- Heat exchange with the atmosphere.

▸ Show problem

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Initial conditions

Obtained by assuming that all the water sources are mixed proportionally to their volume during the first time interval for which they are available.

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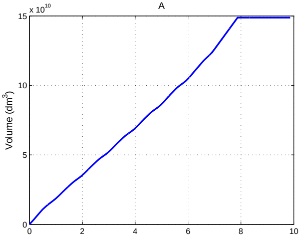
Integration time



Initial conditions

Obtained by assuming that all the water sources are mixed proportionally to their volume during the first time interval for which they are available.

A geochemical example: Numerical results

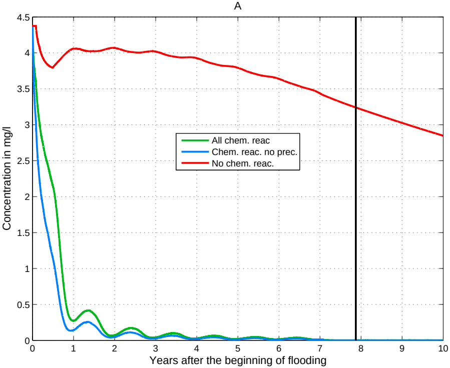
We show the results of a sensitivity test to analyze the effect of the slow chemical reactions and the solubility reactions

- Red line: Results of a simulation in which neither slow nor solubility chemical reactions are considered, just homogeneous equilibria.
- Blue line: Slow and homogeneous reactions but no precipitation are taken into account.
- Green line: Complete geochemical problem.

Results are shown for species that are relevant in mining environments. Fe^{2+}, Fe^{3+}, Al^{3+}, $Alunite$, Mn^{2+} and pH.

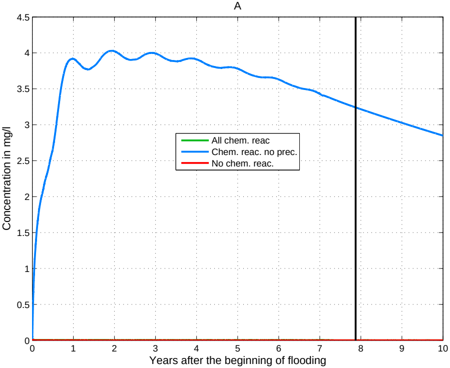
A geochemical example: Numerical results

Ferrous ion



Legal limit: 2mg/l

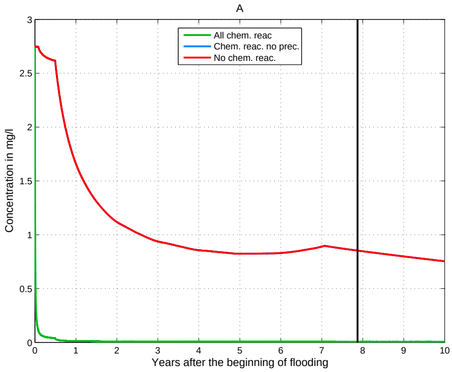
Ferric ion



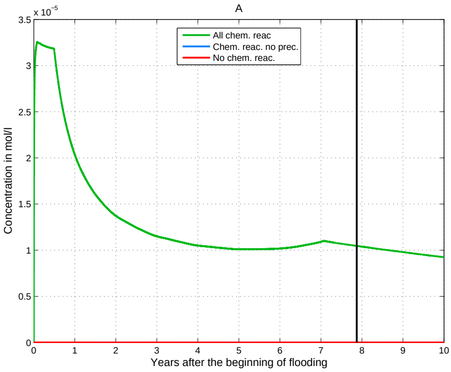
Legal limit: 2mg/l

A geochemical example: Numerical results

Aluminium



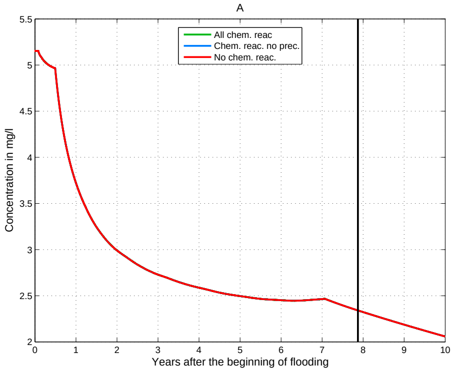
Alunite



Legal limit: 1mg/l

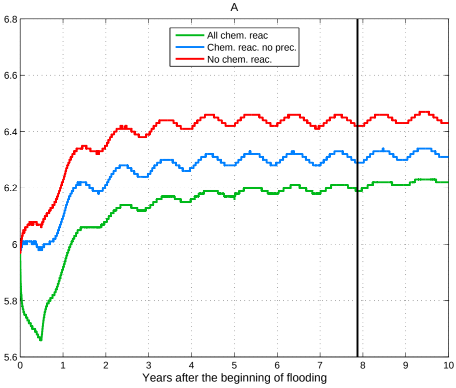
A geochemical example: Numerical results

Manganese



Legal limit: 2mg/l

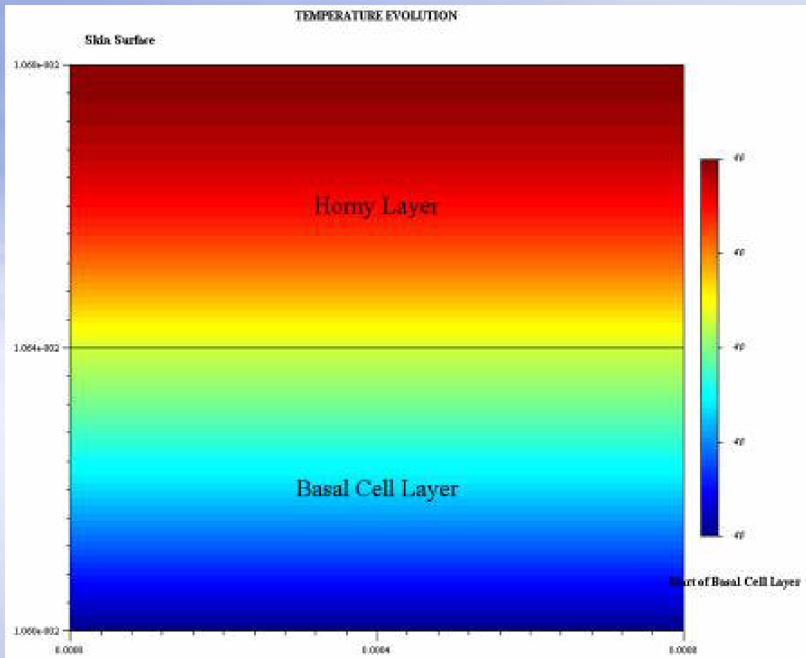
pH



Legal limit: 5.5-9

Daños en tejidos

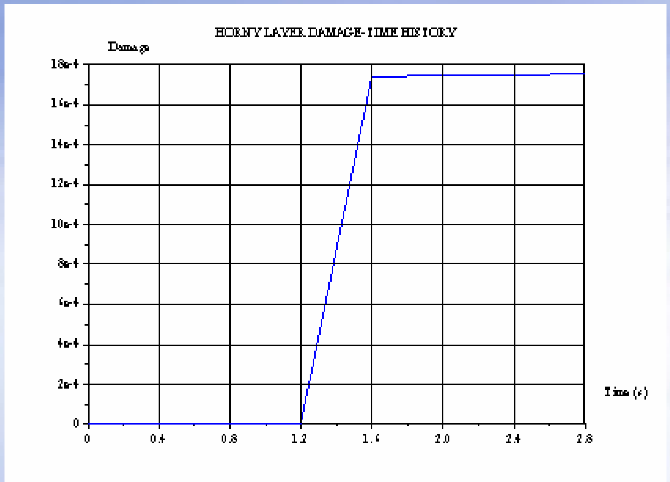
El problema: evaluar el riesgo de quemaduras en la piel como consecuencia de la explosión de un airbag



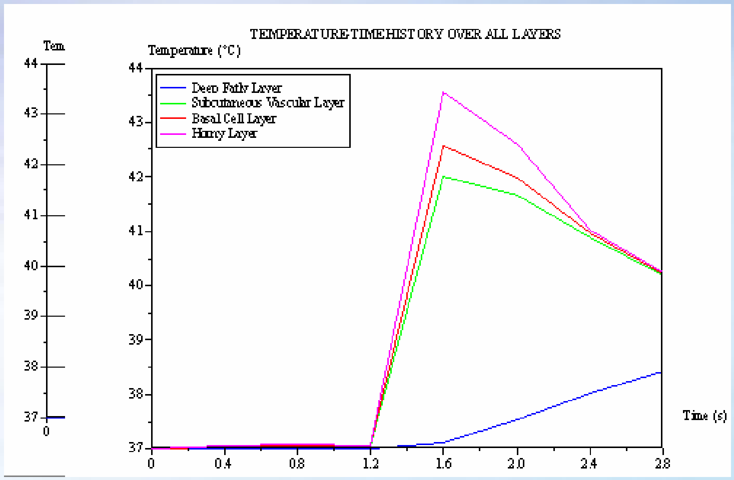
Evolución de la temperaturas sobre las cuatro capas

Daños en tejidos

Objetivos: clasificar la quemadura producida a partir de la evolución de las temperaturas en las distintas capas de la piel



Evolución del daño con respecto al tiempo en el punto más externo del estrato córneo



Evolución de las temperaturas en los puntos más internos de cada una de las capas

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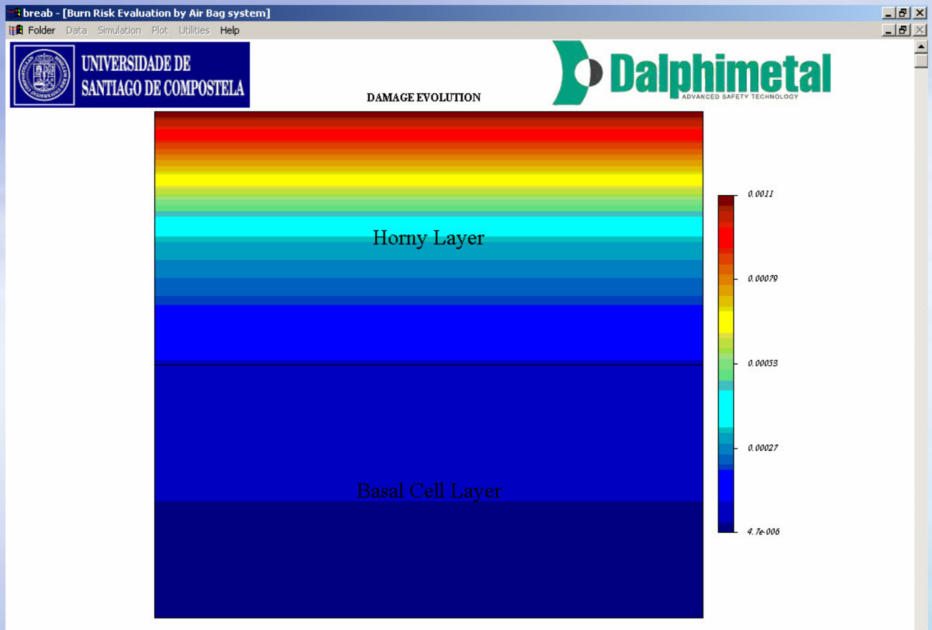
Daños en tejidos

Resultados: elaboración de la aplicación BREAB, que permite determinar la evolución de la temperatura en la piel, simular el daño en los tejidos y clasificar la quemadura producida



Ventana principal de la aplicación BREAB

Proyectos
Líneas

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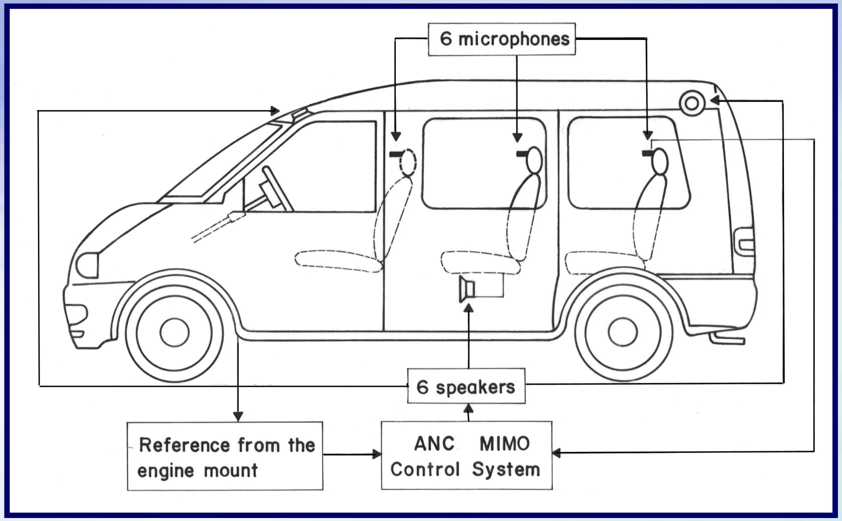
Elastoacústica

El problema: cálculo de vibraciones de un problema de acústica estructural y control activo del ruido



Ejemplo experimental de un problema de control activo de ruido

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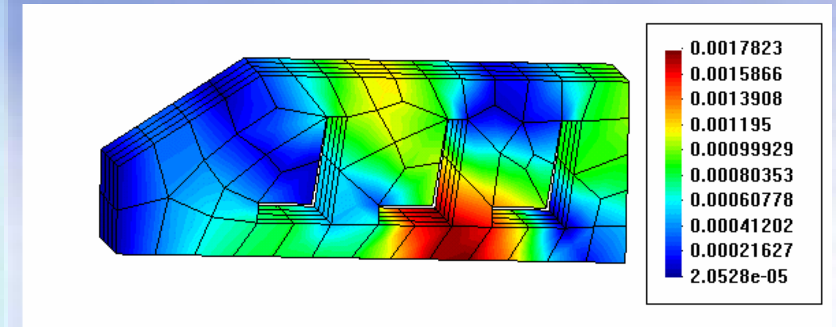
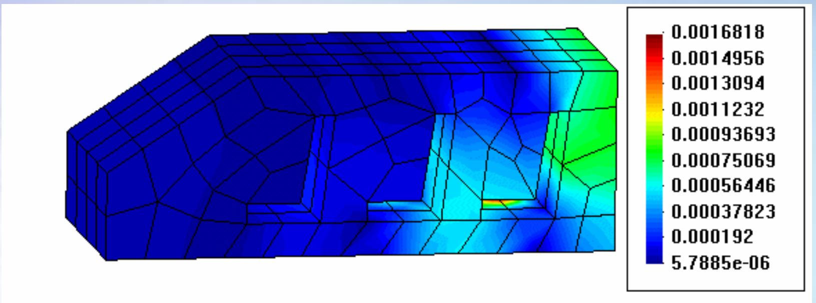
Elastoacústica

Objetivos: elaborar códigos para el cálculo numérico de vibraciones elastoacústicas y resolver problemas de control activo de ruido



Visualización del campo de presiones en el fluido antes del Control activo de ruido



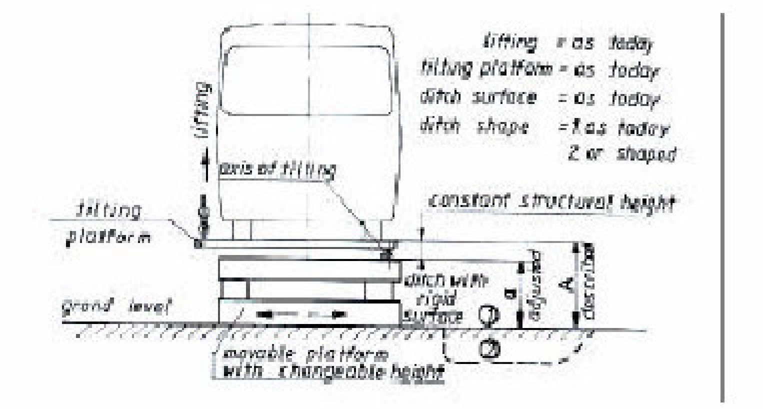
Visualización del campo de presiones en el fluido después del Control activo de ruido

USC UNIVERSIDADE DE SANTIAGO DE COMPOSTELA

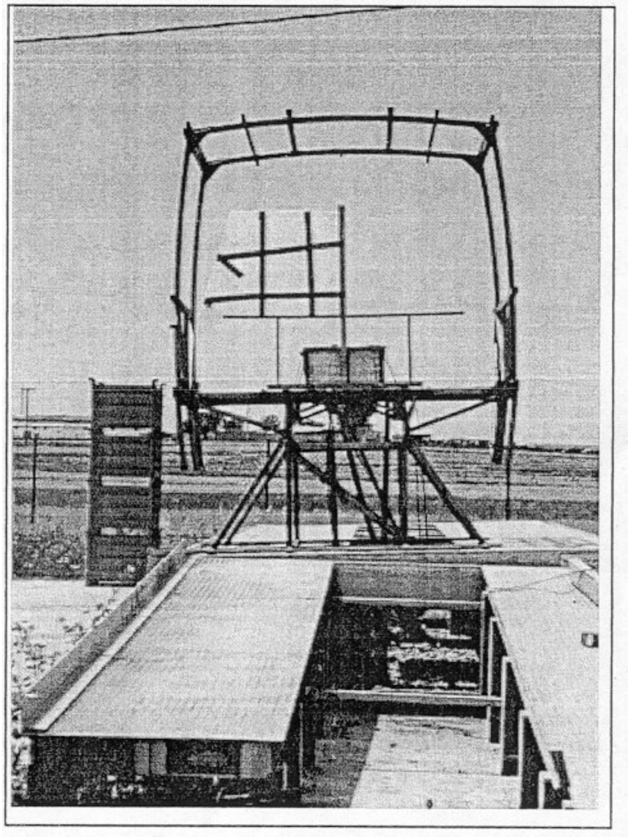
Título: Resistencia estructural y al vuelco de un autobús.
Empresa: Unidad de Vehículos Industriales S. A. (UNVI).
Descripción: Se trata de simular numéricamente las pruebas de resistencia estructural y resistencia al vuelco de un autobús sometido a las cargas contempladas en la correspondiente normativa europea para su legalización.

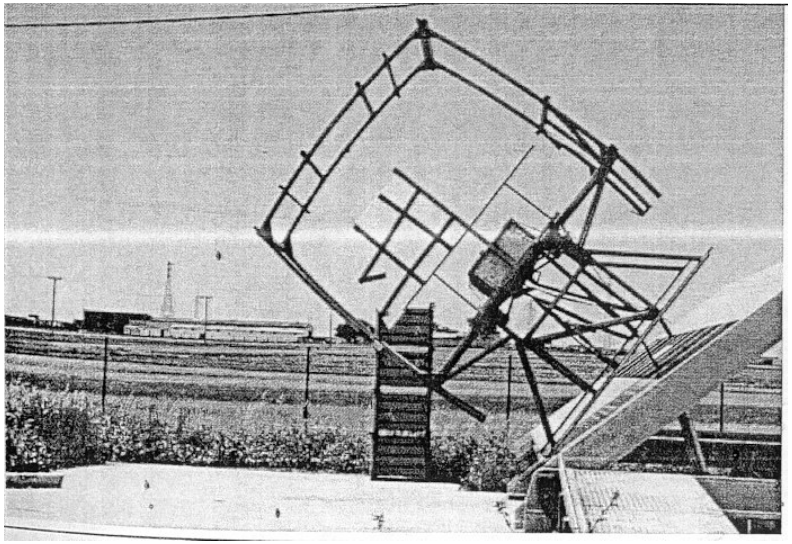
Homologación vehículos de pasajeros: 66R00 sobre resistencia al vuelco.

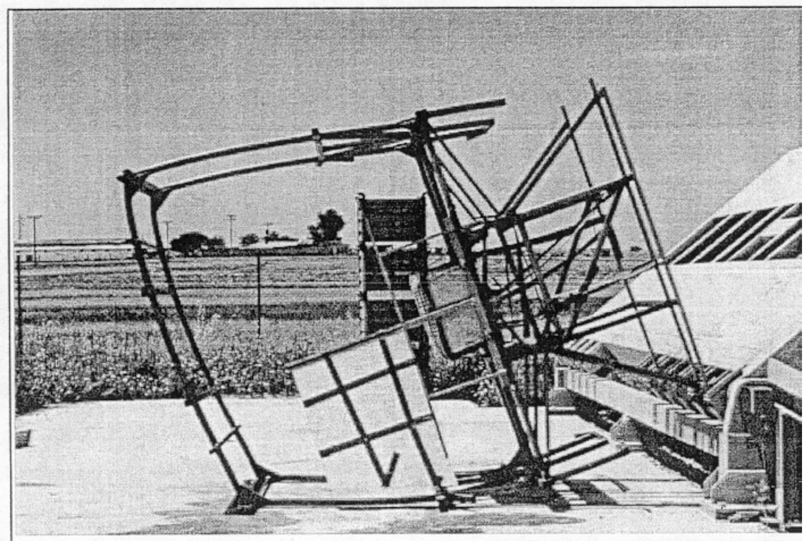
- Servicio Técnico
  - Vehículo completo
  - Secciones superestructura
  - Cálculos numéricos

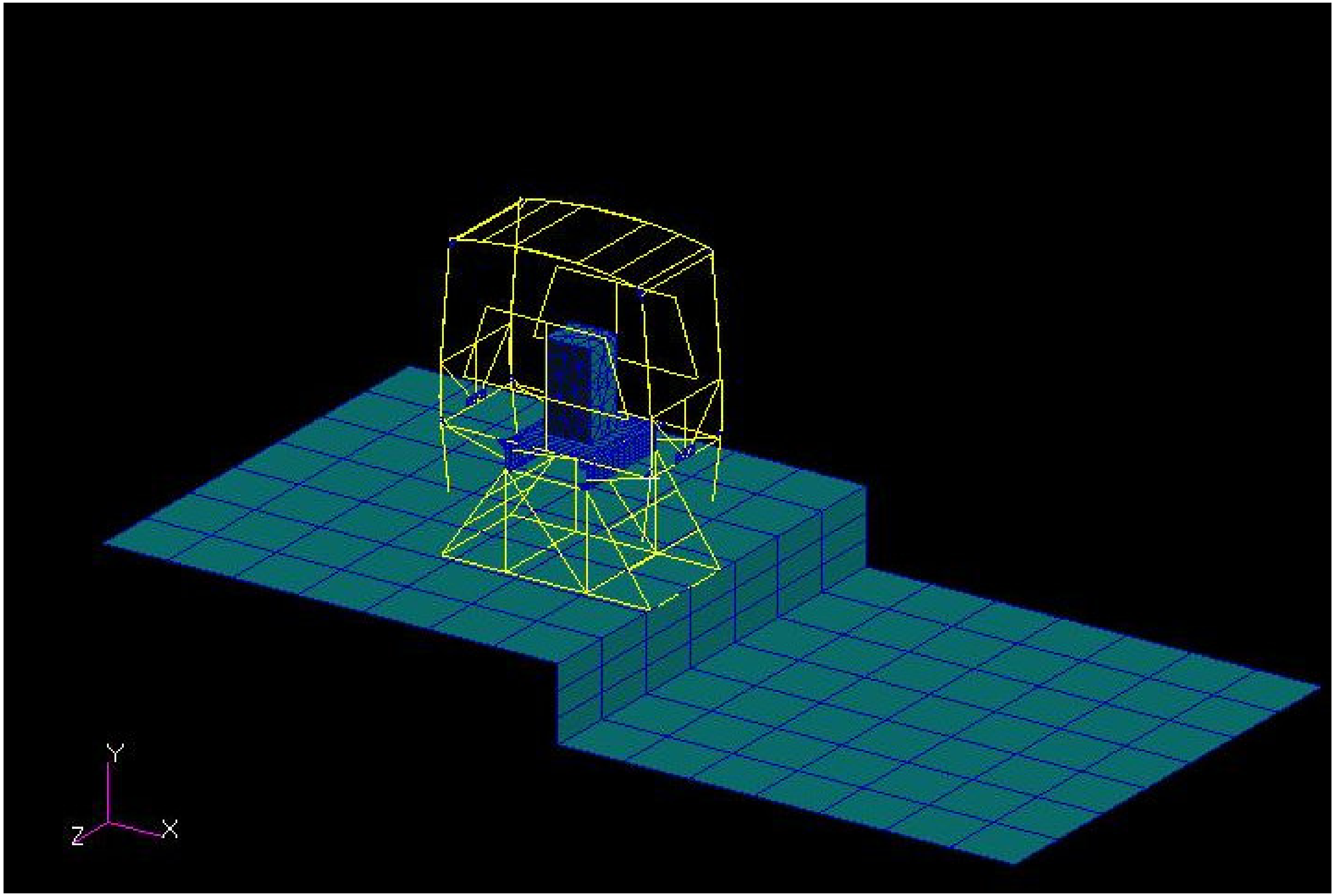


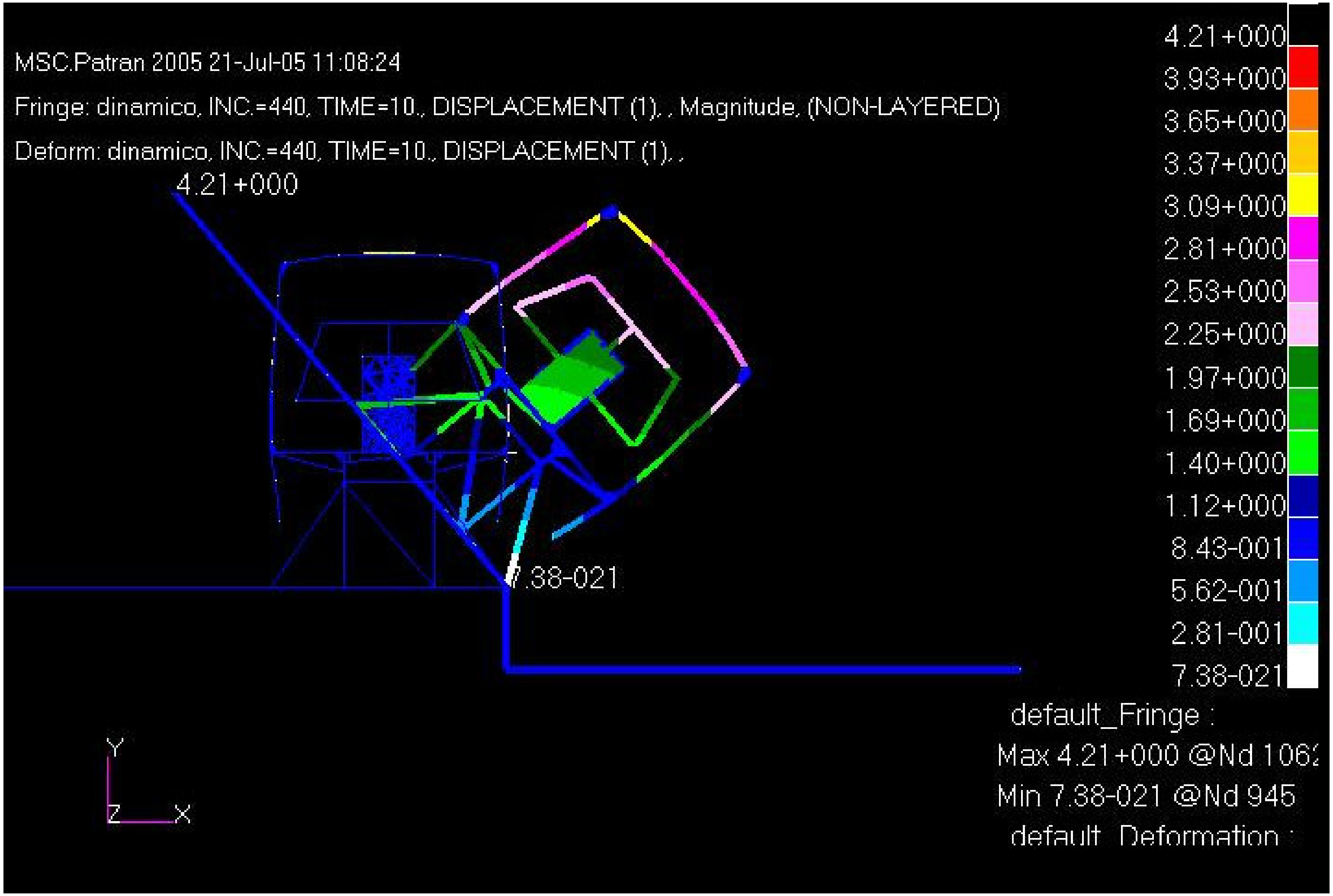
Resistencia al vuelco








Y
Z
X


MSC.Patran 2005 21-Jul-05 11:08:24
Fringe: dinamico, INC.=440, TIME=10., DISPLACEMENT (1), , Magnitude, (NON-LAYERED)
Deform: dinamico, INC.=440, TIME=10., DISPLACEMENT (1), ,
4.21+000
7.38-021
4.21+000
3.93+000
3.65+000
3.37+000
3.09+000
2.81+000
2.53+000
2.25+000
1.97+000
1.69+000
1.40+000
1.12+000
8.43-001
5.62-001
2.81-001
7.38-021
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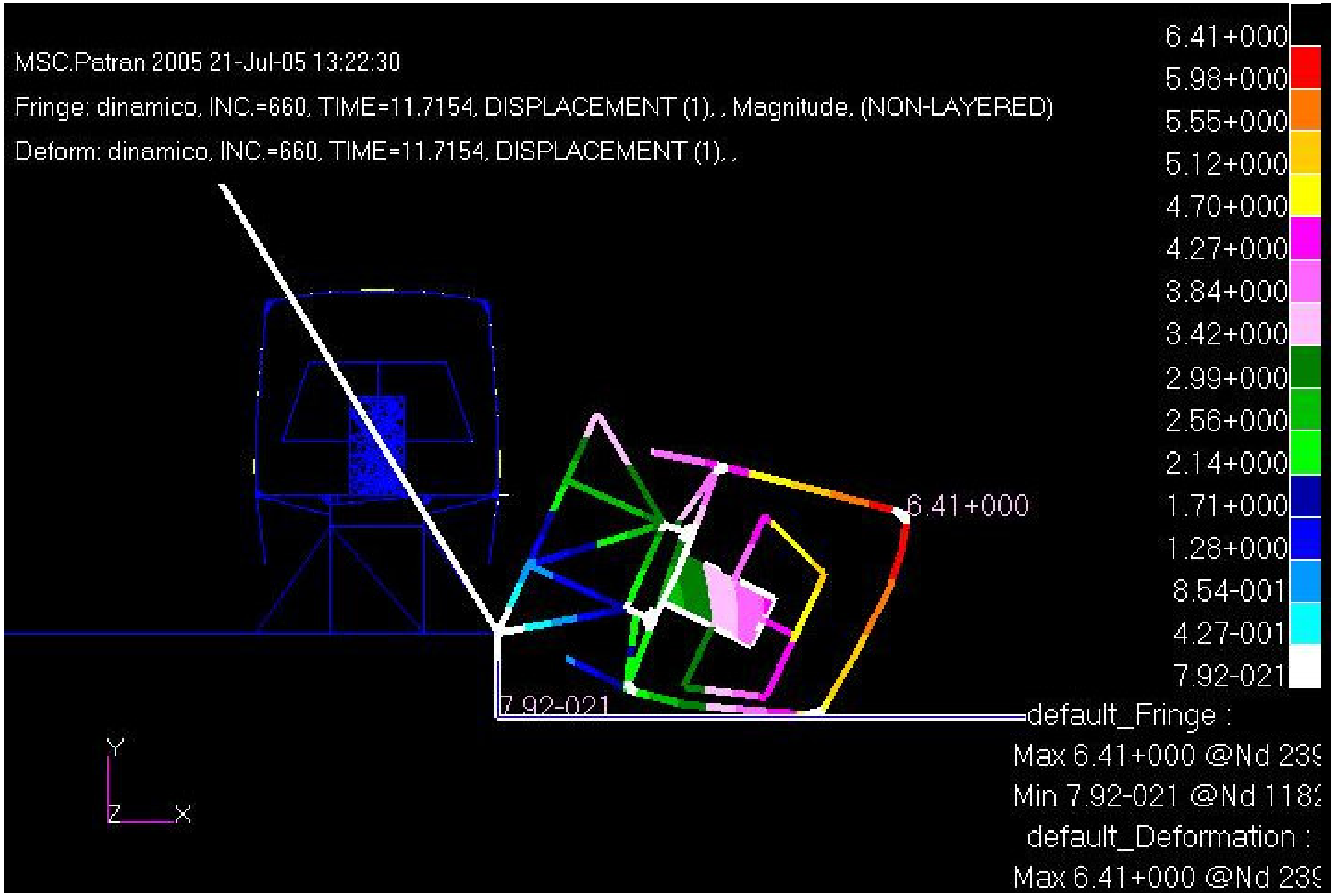
X

Resistencia al vuelco



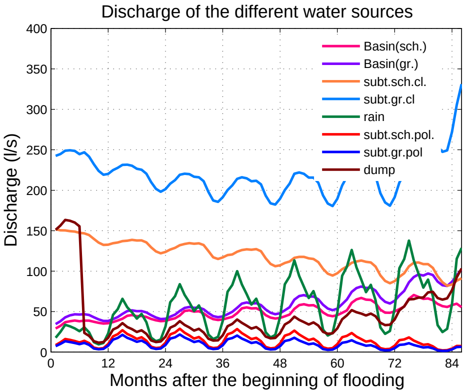
R. idx.(l)	Chemical reaction	Eq. cte.	R. type
16	$H^{+} + SO_4^{2-} \leftrightharpoons HSO_4^{-}$	K_1^e	he
17	$Na^{+} + SO_4^{2-} \leftrightharpoons NaSO_4^{-}$	K_2^e	he
18	$K^{+} + SO_4^{2-} \leftrightharpoons KSO_4^{-}$	K_3^e	he
19	$Mg^{2+} + H_2O - H^{+} \leftrightharpoons MgOH^{+}$	K_4^e	he
20	$Mg^{2+} + SO_4^{2-} \leftrightharpoons MgSO_4$	K_5^e	he
21	$Ca^{2+} + H_2O - H^{+} \leftrightharpoons CaOH^{+}$	K_6^e	he
22	$Ca^{2+} + H^{+} + SO_4^{2-} \leftrightharpoons CaHSO_4^{+}$	K_7^e	he
23	$Ca^{2+} + SO_4^{2-} \leftrightharpoons CaSO_{4(aq)}$	K_8^e	he
24	$Cu^{2+} + H_2O - H^{+} \leftrightharpoons CuOH^{+}$	K_9^e	he
25	$Cu^{2+} + 2H_2O - 2H^{+} \leftrightharpoons Cu(OH)_{2(aq)}$	K_{10}^e	he
26	$Cu^{2+} + 3H_2O - 3H^{+} \leftrightharpoons Cu(OH)_3^{-}$	K_{11}^e	he
27	$Cu^{2+} + SO_4^{2-} \leftrightharpoons CuSO_{4(aq)}$	K_{12}^e	he
28	$Fe^{2+} + H_2O - H^{+} \leftrightharpoons FeOH^{+}$	K_{13}^e	he
29	$Fe^{2+} + 2H_2O - 2H^{+} \leftrightharpoons Fe(OH)_{2(aq)}$	K_{14}^e	he
30	$Fe^{2+} + SO_4^{2-} \leftrightharpoons FeSO_{4(aq)}$	K_{15}^e	he
31	$Fe^{2+} + H^{+} + SO_4^{2-} \leftrightharpoons FeHSO_4^{+}$	K_{16}^e	he
32	$Fe^{3+} + H_2O - H^{+} \leftrightharpoons FeOH^{2+}$	K_{17}^e	he
33	$Fe^{3+} + 2H_2O - 2H^{+} \leftrightharpoons Fe(OH)_2^{+}$	K_{18}^e	he
34	$Fe^{3+} + 3H_2O - 3H^{+} \leftrightharpoons Fe(OH)_{3(aq)}$	K_{19}^e	he
35	$Fe^{3+} + 4H_2O - 4H^{+} \leftrightharpoons Fe(OH)_4^{-}$	K_{20}^e	he
36	$Fe^{3+} + SO_4^{2-} \leftrightharpoons FeSO_4^{+}$	K_{21}^e	he
37	$Fe^{3+} + H^{+} + SO_4^{2-} \leftrightharpoons FeHSO_4^{2+}$	K_{22}^e	he
38	$Fe^{3+} + 2SO_4^{2-} \leftrightharpoons Fe(SO_4)_2^{-}$	K_{23}^e	he
39	$Al^{3+} + H_2O - H^{+} \leftrightharpoons AlOH^{2+}$	K_{24}^e	he
40	$Al^{3+} + 2H_2O - 2H^{+} \leftrightharpoons Al(OH)_2^{+}$	K_{25}^e	he

R. idx.(l)	Chemical reaction	Eq. cte.	R. type
41	$Al^{3+} + 3H_2O - 3H^+ \leftrightharpoons Al(OH)_{3(aq)}$	K^e_{26}	he
42	$Al^{3+} + 4H_2O - 4H^+ \leftrightharpoons Al(OH)_4^-$	K^e_{27}	he
43	$Al^{3+} + H^+ + SO_4^{2-} \leftrightharpoons AlHSO_4^{2+}$	K^e_{28}	he
44	$Al^{3+} + SO_4^{2-} \leftrightharpoons AlSO_4^+$	K^e_{29}	he
45	$Al^{3+} + 2SO_4^{2-} \leftrightharpoons Al(SO_4)_2^-$	K^e_{30}	he
46	$Mn^{2+} + H_2O \leftrightharpoons MnOH^+ + H^+$	K^e_{31}	he
47	$Mn^{2+} + SO_4^{2-} \leftrightharpoons MnSO_4$	K^e_{32}	he
48	$CO_3^{2-} + 2H^+ \leftrightharpoons CO_2 + H_2O\ \ (H_2CO_3)$	K^e_{33}	he
49	$H^+ + CO_3^{2-} \leftrightharpoons HCO_3^-$	K^e_{34}	he
50	$Na^+ + CO_3^{2-} \leftrightharpoons NaCO_3^-$	K^e_{35}	he
51	$Na^+ + HCO_3^- \leftrightharpoons NaHCO_3$	K^e_{36}	he
52	$Mg^{2+} + CO_3^{2-} \leftrightharpoons MgCO_3$	K^e_{37}	he
53	$Mg^{2+} + HCO_3^- \leftrightharpoons MgHCO_3^+$	K^e_{38}	he
54	$Ca^{2+} + CO_3^{2-} \leftrightharpoons CaCO_3$	K^e_{39}	he
55	$Ca^{2+} + HCO_3^- \leftrightharpoons CaHCO_3^+$	K^e_{40}	he
56	$Cu^{2+} + CO_3^{2-} \leftrightharpoons CuCO_3$	K^e_{41}	he
57	$Fe^{2+} + HCO_3^- \leftrightharpoons FeHCO_3^+$	K^e_{42}	he
58	$Fe^{2+} + CO_3^{2-} \leftrightharpoons FeCO_3$	K^e_{43}	he
59	$Mn^{2+} + HCO_3^- \leftrightharpoons MnHCO_3^+$	K^e_{44}	he
60	$Mn^{2+} + CO_3^{2-} \leftrightharpoons MnCO_3$	K^e_{45}	he
61	$H^+ + F^- \leftrightharpoons HF$	K^e_{46}	he
62	$H^+ + 2F^- \leftrightharpoons HF_2^-$	K^e_{47}	he
63	$Na^+ + F^- \leftrightharpoons NaF$	K^e_{48}	he
64	$Mg^{2+} + F^- \leftrightharpoons MgF^+$	K^e_{49}	he
65	$Ca^{2+} + F^- \leftrightharpoons CaF^+$	K^e_{50}	he
66	$Cu^{2+} + F^- \leftrightharpoons CuF^+$	K^e_{51}	he

R. idx.(l)	Chemical reaction	Eq. cte.	R. type
67	$Fe^{2+} + F^{-} \leftrightharpoons FeF^{+}$	K^e_{52}	he
68	$Fe^{3+} + F^{-} \leftrightharpoons FeF^{2+}$	K^e_{53}	he
69	$Fe^{3+} + 2F^{-} \leftrightharpoons FeF_2^{+}$	K^e_{54}	he
70	$Fe^{3+} + 3F^{-} \leftrightharpoons FeF_3$	K^e_{55}	he
71	$Al^{3+} + F^{-} \leftrightharpoons AlF^{2+}$	K^e_{56}	he
72	$Al^{3+} + 2F^{-} \leftrightharpoons AlF_2^{+}$	K^e_{57}	he
73	$Al^{3+} + 3F^{-} \leftrightharpoons AlF_3$	K^e_{58}	he
74	$Al^{3+} + 4F^{-} \leftrightharpoons AlF_4^{-}$	K^e_{59}	he
75	$Mn^{2+} + F^{-} \leftrightharpoons MnF^{+}$	K^e_{60}	he
76	$Cu^{2+} + Cl^{-} \leftrightharpoons CuCl^{+}$	K^e_{61}	he
77	$Cu^{2+} + 2Cl^{-} \leftrightharpoons CuCl_2$	K^e_{62}	he
78	$Cu^{2+} + 3Cl^{-} \leftrightharpoons CuCl_3^{-}$	K^e_{63}	he
79	$Cu^{2+} + 4Cl^{-} \leftrightharpoons CuCl_4^{2-}$	K^e_{64}	he
80	$Fe^{2+} + Cl^{-} \leftrightharpoons FeCl^{+}$	K^e_{65}	he
81	$Fe^{3+} + Cl^{-} \leftrightharpoons FeCl^{2+}$	K^e_{66}	he
82	$Fe^{3+} + 2Cl^{-} \leftrightharpoons FeCl_2^{+}$	K^e_{67}	he
83	$Fe^{3+} + 3Cl^{-} \leftrightharpoons FeCl_3$	K^e_{68}	he
84	$Mn^{2+} + Cl^{-} \leftrightharpoons MnCl^{+}$	K^e_{69}	he
85	$Mn^{2+} + 2Cl^{-} \leftrightharpoons MnCl_2$	K^e_{70}	he
86	$Mn^{2+} + 3Cl^{-} \leftrightharpoons MnCl_3^{-}$	K^e_{71}	he
87	$H_2O - H^{+} \leftrightharpoons OH^{-}$	K^e_{72}	he
88	$Fe(OH)_3 - 6L + 3H^{+} \leftrightharpoons Fe^{3+} + 3H_2O$	K^s_1	mp
89	$KAl_3(SO_4)_2(OH)_6 + 6H^{+} \leftrightharpoons K^{+} + 3Al^{3+} + 2SO_4^{2-} + 6H_2O$	K^s_2	mp
90	$MnOOH + 3H^{+} \leftrightharpoons Mn^{2+} + 2H_2O$	K^s_3	mp
91	$CaSO_4.2H_2O \leftrightharpoons Ca^{2+} + SO_4^{2-} + 2H_2O$	K^s_4	mp

R. idx.(l)	Chemical reaction	Eq. cte.	R. type
92	$HFO-sOH + H^{+} \leftrightharpoons HFO-sOH_2^{+}$	K_1^a	ad
93	$HFO-sOH \leftrightharpoons HFO-sO^{-} + H^{+}$	K_2^a	ad
94	$HFO-sOH + Ca^{2+} \leftrightharpoons HFO-sOCa^{+} + H^{+}$	K_3^a	ad
95	$HFO-sOH + Cu^{2+} \leftrightharpoons HFO-sOCu^{+} + H^{+}$	K_4^a	ad
96	$HFO-sOH + Mn^{2+} \leftrightharpoons HFO-sOMn^{+} + H^{+}$	K_5^a	ad
97	$HFO-sOH + Fe^{2+} \leftrightharpoons HFO-sOFe^{+} + H^{+}$	K_6^a	ad
98	$HFO-wOH + H^{+} \leftrightharpoons HFO-wOH_2^{+}$	K_7^a	ad
99	$HFO-wOH \leftrightharpoons HFO-wO^{-} + H^{+}$	K_8^a	ad
100	$HFO-wOH + Ca^{2+} \leftrightharpoons HFO-wOCa^{+} + H^{+}$	K_9^a	ad
101	$HFO-wOH + Cu^{2+} \leftrightharpoons HFO-wOCu^{+} + H^{+}$	K_{10}^a	ad
102	$HFO-wOH + Mg^{2+} \leftrightharpoons HFO-wOMg^{+} + H^{+}$	K_{11}^a	ad
103	$HFO-wOH + Mn^{2+} \leftrightharpoons HFO-wOMn^{+} + H^{+}$	K_{12}^a	ad
104	$HFO-wOH + Fe^{2+} \leftrightharpoons HFO-wOFe^{+} + H^{+}$	K_{13}^a	ad
105	$HFO-wOH + SO_4^{2-} + H^{+} \leftrightharpoons HFO-wSO_4^{-} + H_2O$	K_{14}^a	ad
106	$HFO-wOH + SO_4^{2-} \leftrightharpoons HFO-wOHSO_4^{2-}$	K_{15}^a	ad
107	$HFO-wOH + F^{-} + H^{+} \leftrightharpoons HFO-wF + H_2O$	K_{16}^a	ad
108	$HFO-wOH + F^{-} \leftrightharpoons HFO-wOHF$	K_{17}^a	ad
109	$HFO-wOH + CO_3^{2-} + H^{+} \leftrightharpoons HFO-wCO_3^{-} + H_2O$	K_{18}^a	ad
110	$HFO-wOH + CO_3^{2-} + 2H^{+} \leftrightharpoons HFO-wHCO_3 + H_2O$	K_{19}^a	ad

- The **discharge** of the 8 water sources is known.



- The **water quality** was measured in the field.

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$$
\mathcal{P}_{st}
\begin{cases}
\frac{d\mathbf{y}}{dt}(t) = \mathbf{f}^{y}(t, \mathbf{y}(t)) + \mathcal{A}^{e}\mathbf{p}^{e}(t) + \mathcal{A}^{s}\mathbf{p}^{s}(t) + \mathcal{A}^{a}\mathbf{p}^{a}(t) + \frac{1}{V(t)}\big(\phi^{y,b}(t, \mathbf{y}(t))\mathbf{S}^{b}(t) \\
+\varphi^{y,a}(t, \mathbf{y}(t))S^{a}(t)\big) + \frac{1}{V(t)}\big(\mathsf{A}(t)\mathbf{q}(t)\big), & (5) \\
\mathbf{g}^{e}(t, \mathbf{y}(t), \theta(t), I(t)) = \mathbf{0}, & (6) \\
\mathbf{g}^{s}(t, \mathbf{y}(t), \theta(t), I(t)) \leq \mathbf{0}, & (7) \\
\mathbf{p}^{s}(t) \geq \mathbf{0}, & (8) \\
\mathbf{g}^{s}(t, \mathbf{y}(t), \theta(t), I(t))\mathbf{p}^{s}(t) = \mathbf{0}, & (9) \\
\mathbf{g}^{a}(t, \mathbf{y}(t), \theta(t), I(t), \mathbf{P}(t)) = \mathbf{0}, & (10) \\
I(t) = \frac{1}{2}(\mathbf{cc}) \cdot \mathbf{y}(t), & (11) \\
\boldsymbol{\sigma}(\mathbf{y}(t)) = \frac{0.1174 I(t)^{1/2}}{2}\hat{\mathbf{P}}(t), & (12) \\
\frac{d\theta}{dt}(t) = \frac{1}{V(t)\left(\rho(t) + \theta(t)\frac{\partial\hat{\rho}(\theta(t))}{\partial\theta(t)}\right)}\Bigg[(\boldsymbol{\rho}(t)\boldsymbol{\theta}(t)) \cdot \mathbf{q}(t) - \rho(t)\theta(t)q_0(t) - \theta(t)\Bigg(V(t)\Big(\sum_{i=1}^{N} M_i \frac{dy_i(t)}{dt}\Big) \\
+\rho(t)\Big(\sum_{j=1}^{N^s} q_j(t) - q_0(t)\Big)\Bigg) + \frac{S^a(t)}{C_e}Q_{atm}(t, \theta(t))\Bigg], & (13) \\
\frac{dV(t)}{dt} = \sum_{j=1}^{N^s} q_j(t) - q_0(t), & (14) \\
\mathbf{y}(0) = \mathbf{y}_{init}, & (15) \\
\theta(0) = \theta_{init}, & (16) \\
V(0) = V_{init}, & (17)
\end{cases}
$$

Number of chemical reactions of each kind

1, 72, 4, 19, 12, 1

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