A SULFIDE-DRIVEN FUEL CELL:
THE CATHODE CELL WITH EJECTOR MIXER
Part 2. Double density mesh

The institute of Chemical Engineering in Sofia

Keywords

FC, ORR, CFD, visualization, velocity distribution, ϵ-distribution related to mass transfer

(ϵ = rate of energy dissipation rate)

Main topics

- **Introduction** — Driving force of the study
- **Aim of this study** — A global and a more specific one
- **Cathode chamber design**
- **Methods** CFD — Numerical model and procedure
- **Results** — Characteristics of the ejector cell

  Overview of previous results ***(refreshment)***

  Framework of a further study

  Mesh refinement results

- **In conclusion** — Further cell geometry

Introduction

Driving forces of the study

- **There are just a few studies on the problem**
- Development of a **technical-scale process**

Aims of the study

Global aim

Development of a technical-scale process

More specific aims

(1) To formulate a flow model of the cathode cell and

(2) To characterize the flow field in view of increasing the cell potential for enhanced oxygen reduction.

Stages of analysis for the cathode cycle Focus on reactaint transport

Basic Fuel Cell Operation

1.Reactant transport

- Efficient delivery of reactants - **local flow field and mass transfer around the electrode structures** (plates or cylinders in combination with porous electrodes) It is important to ensure active access to the electrode surface

2.Electrochemical reaction

- Choosing right catalyst and **carefully designing reaction zones**

3.Ionic (and Electronic) Conduction

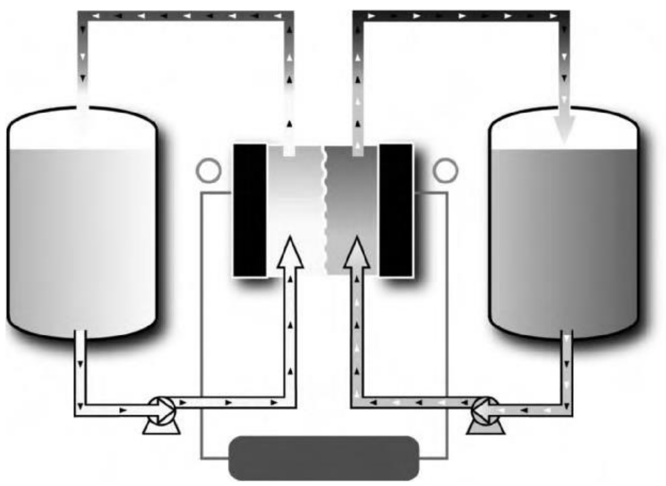
- Thin electrolyte for ionic conduction, without fuel cross over

4.Product Removal

- •"Flooding" by product water can be major issue of the cell

Global aim illustrated by an example

Focus on the sulfide-driven power plant “Regenesis Technol.”



a solution of sodium sulphide (Na_2S_2) in water is fed to the negative electrode

a sodium tribromide ($NaBr_3$) solution is fed to the positive electrode

$2Na_2S_2 \rightarrow Na_2S_4 + 2Na^+ + 2e^-$

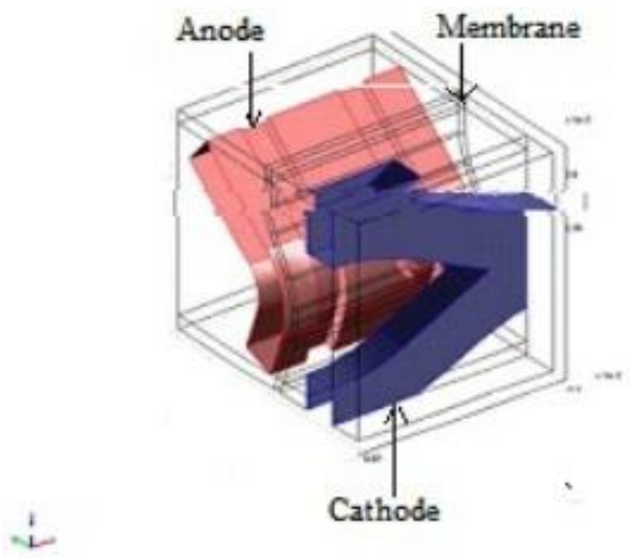
$NaBr_3 + 2Na^+ + 2e^- \rightarrow 3NaBr$

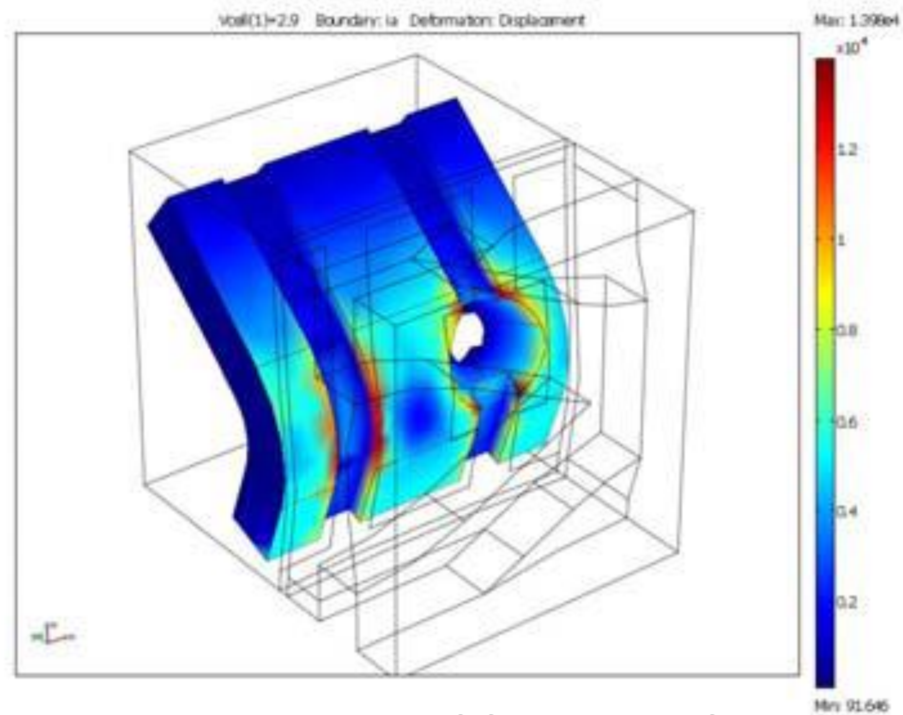
Picture of the 100-MWh electrical energy storage facility being installed in Cambridgeshire,England.

An Introduction to Electrochemical Power Sources

Author(s):
C.A. Vincent and B Scrosati
ISBN: 978-0-340-66278-6

Specific aims illustrated by example
Focus on the electrode design





The calculated cell voltages have a precision in the range of few tens of mVs and so are sufficient to predict the correct ranking of the different shapes.

The method has proved to be valid and helpful for saving time and resources

Giuseppe Faita, Angelo Ottaviani: Method for the integration of fuel cells into electrochemical plants. Nuvera Fuel Cells Europe.Jul, 23 2002: US6423203

By the way

THE UNIVERSITY OF CRAIOVA CHEMISTRY FACULTY

Dpl. Eng. Marius Constantin Mirica

Doctoral Thesis

ELECTROCHEMICAL REACTORS WITH ASYMMETRICAL CURRENT DENSITIES

Coordinator: Prof. dr. Mircea PREDA

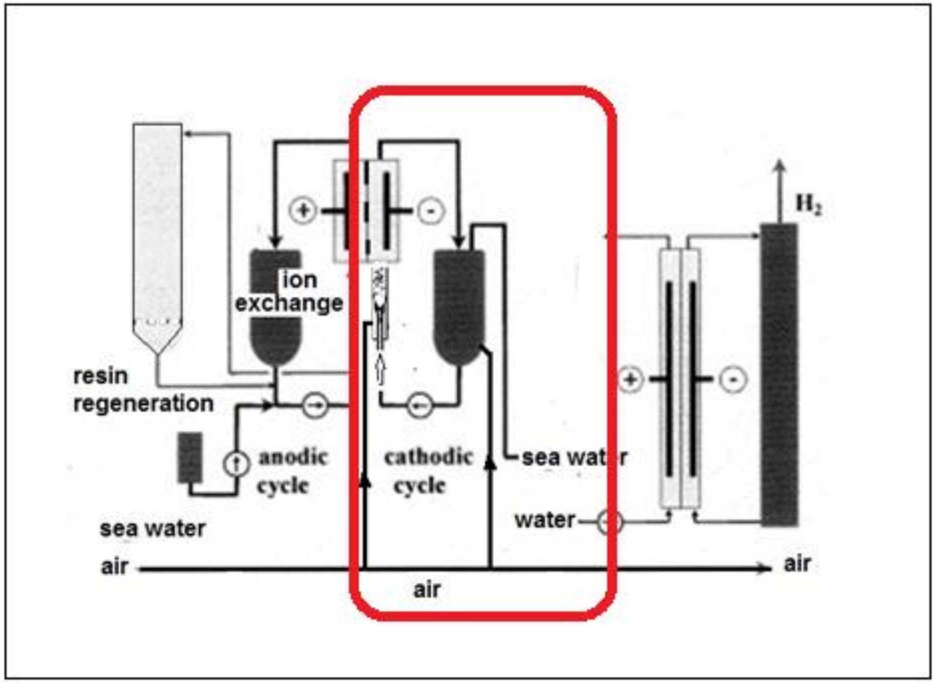
2004

FOLLOWING OUR STUDY

Cathode oxygen reduction reaction (ORR):

$2O_2 + 8H^+ + 8e^- = 4H_2O$.

Focus on the cathode hydrodynamics



A version of a design solution

- **Electrode cell for simultaneous intensive aeration accompanied by oxygen reduction**

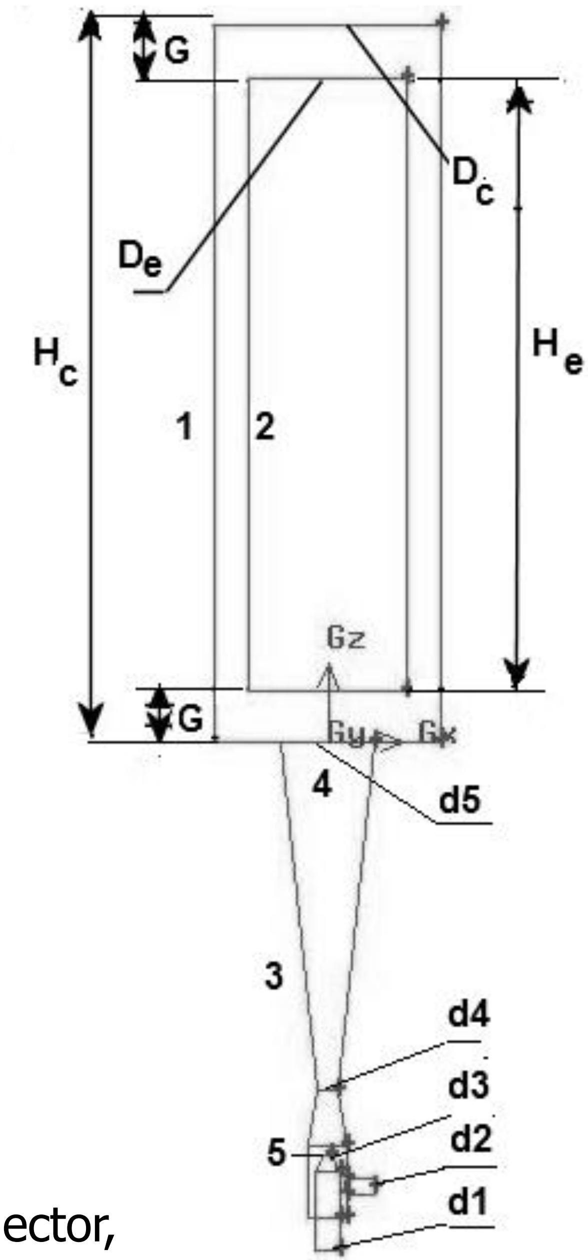
- **A chamber with cylindrical electrode and <u>ejector gas distributor</u>; <u>liquid phase at forced circulation</u> by using a pump**

- **Reference to previous studies showed <u>compatible energy consumption</u>, thus, reasonable application of such a device.**

The cathode chamber

Table 1 Geometry

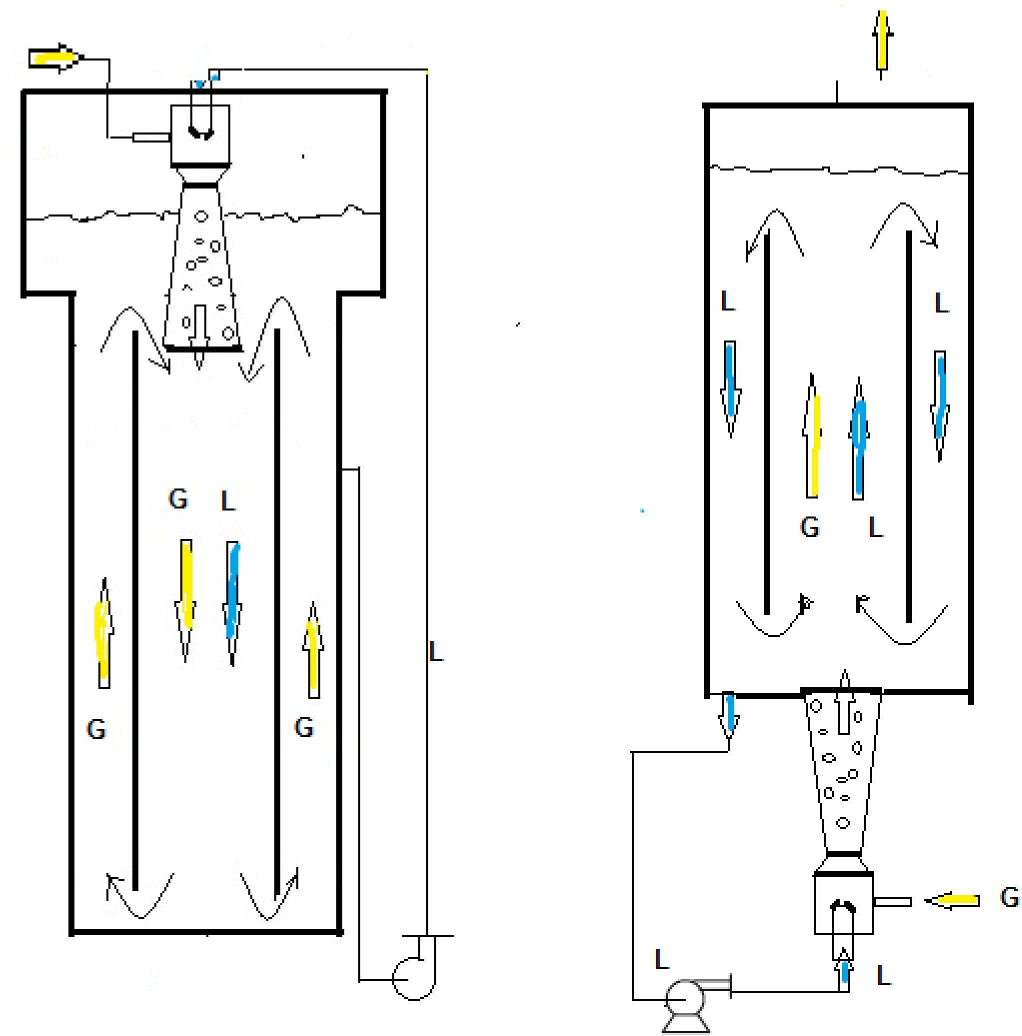
Parameter	Dimension (m)
D_c	0.145
D_e	0.08
d_1	0.015
d_2	0.010
d_3	0.004
d_4	0.015
d_5	0.080
G	0.032
H_c	0.45
H_e	0.385



Ejector and column schematics:
1 is column, 2 cylinder electrode, 3 air ejector,
4 ejector diffuser,5 ejector nozzle.

TWO DESIGN VERSIONS FOR THE EJECTOR

Случай 1 /ляво/: Ежектора отгоре, газ-течностен поток надолу в цилиндричното пространство, отвеждане на газа в горния капак.
Случай 2 /дясно/: Ежектора е отдолу, газо-течностен поток нагоре в цилиндричното пространство, сепарация горе и циркулация ва нечността надолу по периферията
В ежектора: първичен флуид е водата, засмуква се газа, който е вторичен флуид.
Газът се засмуква във входния щуцер на смукалната камера на ежектора, увличан от подналягането, създадено от струята на течностния поток.
Внимание: Обърни внимание на специфичните геометрични параметри на ежектора и техните стойности. Схема е дадена отделно!



A model has to be defined

that takes into account:

1) Full hydrodynamic description (CFD) using the mixture model that accounts of

- Buoyancy effect from the gas content
- Viscosity effects due to gas content
- Relative velocity between the gas phase and the liquid phase

(2) A primary current distribution model (Ohm's law for ionic conduction in the electrolyte domain)

(3) Full electrode kinetic expressions (Butler-Volmer expressions)

[including the influence of both activation and concentration over-potential, where concentration over-potential depends only on an input parameter, the boundary layer thickness, and not on a real salt concentration distribution]

(4) Diffusion-convection equation (full current distribution).

NUMERICAL MODEL AND PROCEDURE

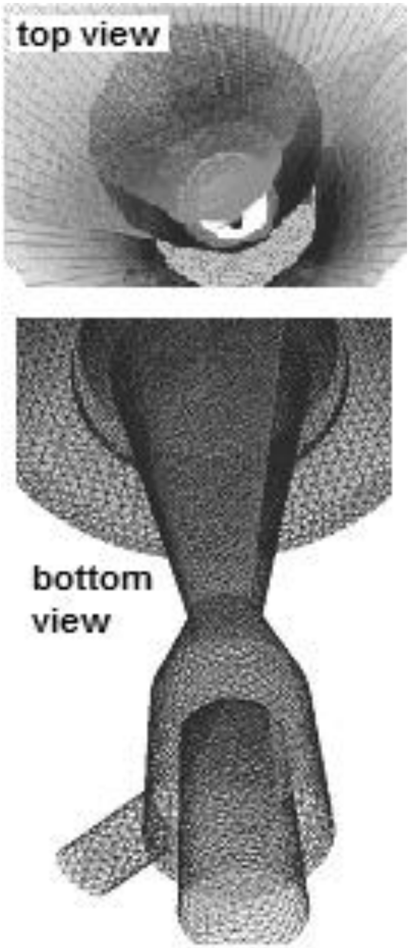
- the continuity equation

$$\frac{\partial}{\partial t}\left(\rho_m\right)+\nabla\cdot(\rho_m U_m)=0$$

- the momentum equation

$$\frac{\partial}{\partial t}(\rho_m U_m)+\nabla\cdot(\rho_m U_m U_m)=-\nabla P+\rho_m g+\nabla\cdot[(\mu_m(\nabla U_m+\nabla U_m^T)]+F+\nabla\cdot(\alpha_L\rho_L\overline{u_{rL}^{'}u_{rL}^{'}}+\alpha_G\alpha_G\overline{u_{rG}u_{rG}})$$

Simulation domain



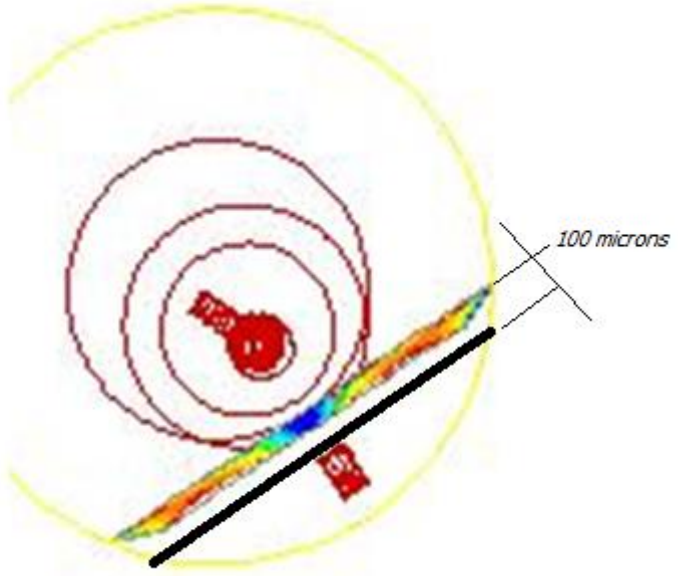
Refreshment over previous results

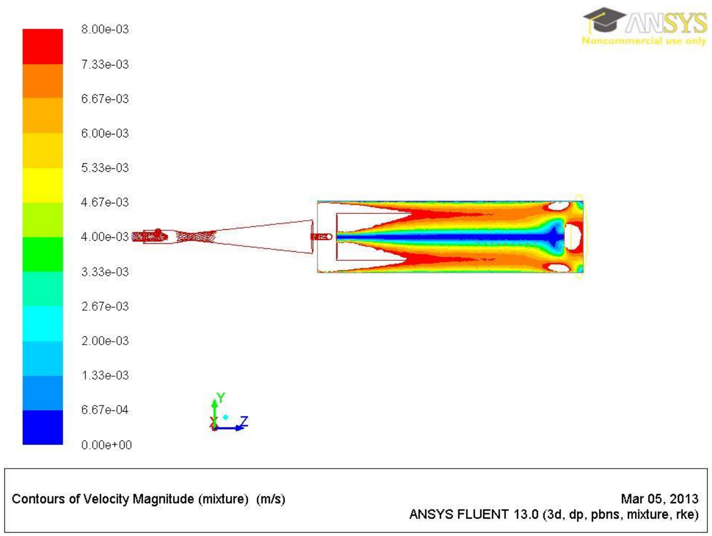
Overview of previous results (refreshment)

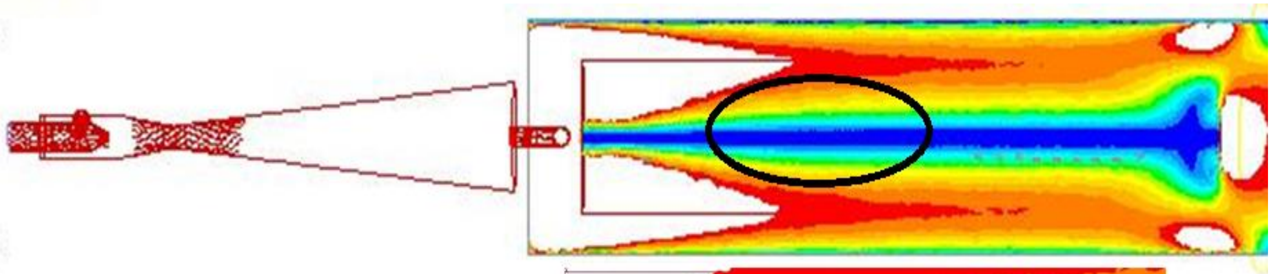
Various computational aspects have been resolved

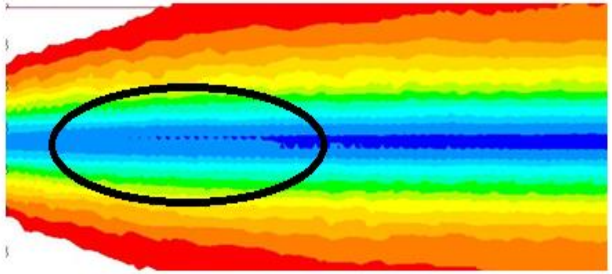
- The conservation equations for mass and momentum has been solved to resolve the convective flows.
- Mesh requirement and parallel computing has been resolved.
- Solution algorithms have been fixed up.
- Velocity vectors and density contours in the cathode channel at different locations have been determined

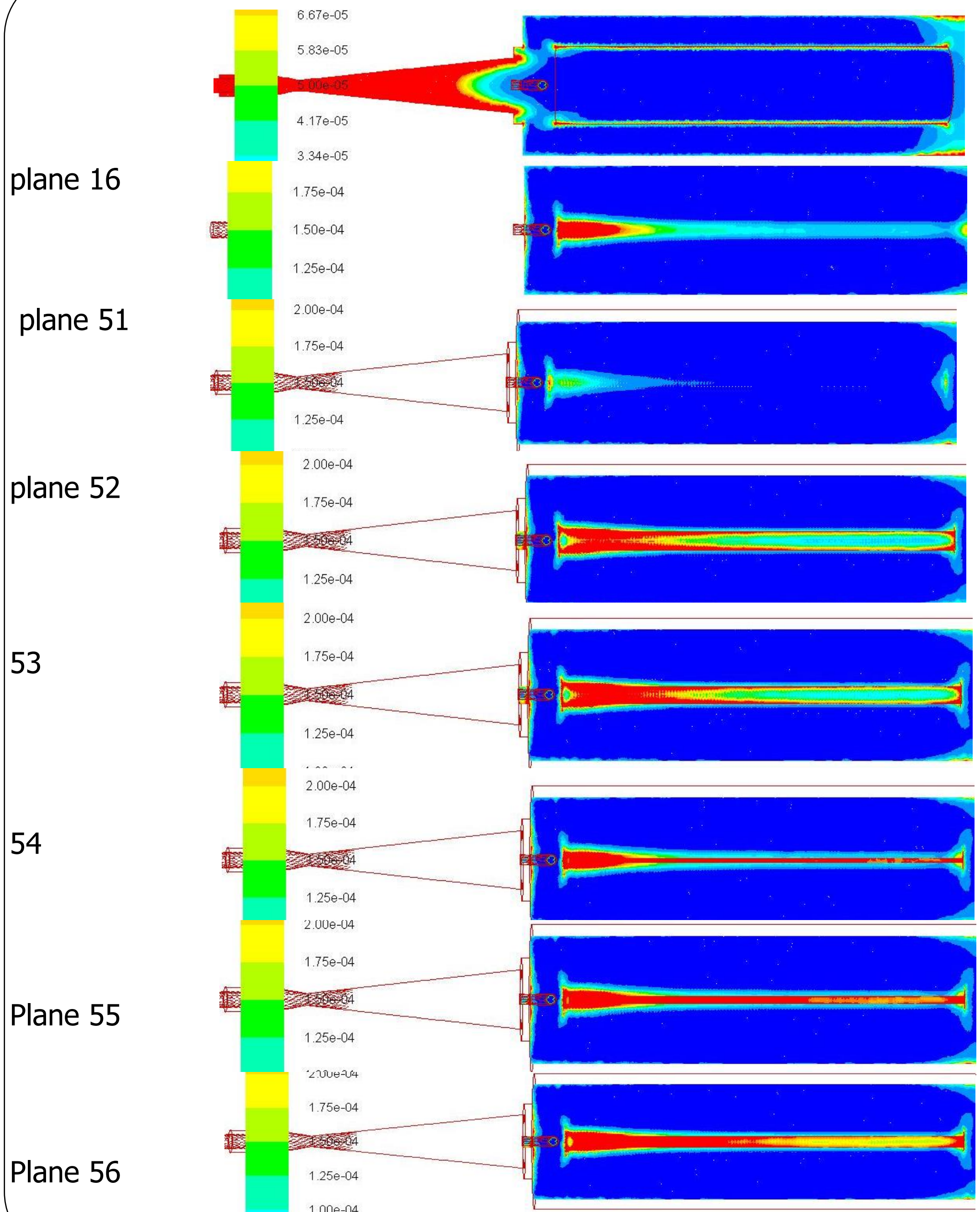
Overview of previous results (refreshment)











Example solution contours over various flat planes

13th International Multidisciplinary Scientific GeoConference

FLOW MODELING OF A SULFIDE-DRIVEN FUEL CELL: THE CATHODE CELL WITH EJECTOR MIXER

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ABSTRACT Oxydation of sulfide from Black Sea water for energy generation by sulfide-driven fuel cell is considered. A serious problem is the slow cathode oxygen reduction reaction (ORR): $2O_2 + 8H^+ + 8e^- = 4H_2O$. A solution is found by designing a cell with forced circulation by means of ejector. A cathode chamber with cylindrical coaxial electrode is proposed. Regarding the transport properties of the cathode area, the flow regime in the cathode compartment is studied. The task is solved by numerical modeling and simulation. The model can be combined with the current distribution model (Ohm's law for ionic conduction), the electrode kinetic expressions (Butler-Volmer) and a diffusion convection equation for the ionic transport and can be implemented for complete description of current distribution and cell voltage thus promoting future analyses of the energy-storage system

Introduction

- Black Sea water contains enormous amount of hydrogen sulfide estimated as **4.6 bill. t** and this amount is increasing progressively.
- The sulfide is a potential source of energy, provided it could be converted by specialized chemical processing.
- It is most convenient to convert chemical energy directly to electrical energy involving electochemical devices.

- **The aim of this study is to formulate a flow model of the cathode cell and to characterize the flow field in view of increasing the cell potential for enhanced oxygen reduction.**

Details of cathode cell design and the model

- The task is solved by numerical modeling and simulation.
- Commercial computational flow dynamics (CFD) software was used.
- A two-phase quasi-homogeneous mixture model is formulated and used in couple with k-ϵ turbulence model.
- For details, see [1, 2].

Table 1 Geometry

Parameter	Dimension (m)
D_c	0.145
D_e	0.08
d_1	0.015
d_2	0.010
d_3	0.004
d_4	0.015
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G	0.032
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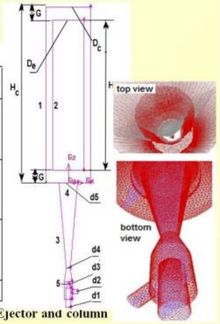
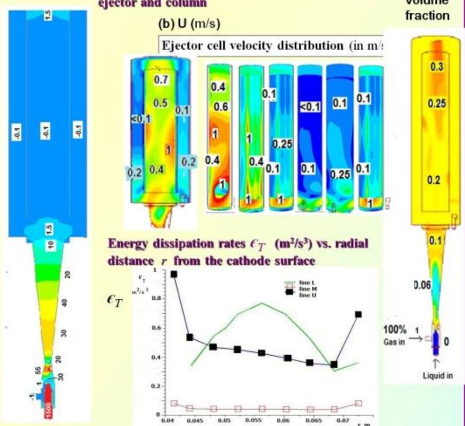


Ejector and column

Results

Pressure p (a, kPa), velocity U (b, m/s) and gas holdup (c) distribution in gas-liquid flow field of ejector and column



Energy dissipation rate ϵ_T in the vessel is increasing strongly and affects oxygen mass transfer by shifting the mass transfer coefficient k_L to larger values according to the equation .The trend is largely observed in the inner cathode area.

$$k_L = \frac{2}{\sqrt{\pi}}\sqrt{D_{ab}}\left(\frac{\epsilon_T \rho}{\eta}\right)^{1/4}$$

Position ε_T m²/s³	1	0.4	0.04	10	100
K_L m/s 10^{-4}	15.6	6.24	0.66	2.7	5

References

[1] Beschkov V. & Razkazova-Velkova E. Utilization of sulfide from Black Sea water by electrolysis, International Journal of Current Chemistry, 1, 7-15, 2010

[2] Kandakure M.T., Gaikar V.G. & Patwardhan A.W. Hydrodynamic aspects of ejectors, Chem, Eng. Sci., 60, 6391-6402, 2005.

Acknowledgement

The study is part of Project HYSULFCEL supported by BS-ERA.NET related to Framework Programme 7.

Conclusions

- A flow model of the cathode compartment of a sulfide-driven fuel cell is formulated and its flow regime is explored.
- The key parameters of the flow field, i.e. static pressure, fluid velocity, phase volume fraction, and kinetic energy dissipation rate are determined
- Prognostic values of the mass transfer coefficient show wide 3-fold **variation** across the cathode surface, namely, **($0.6x10^{-4}$** m/s to **$15.6x10^{-4}$** m/s) and imply strong influence of the flow regime over the ionic diffusion..

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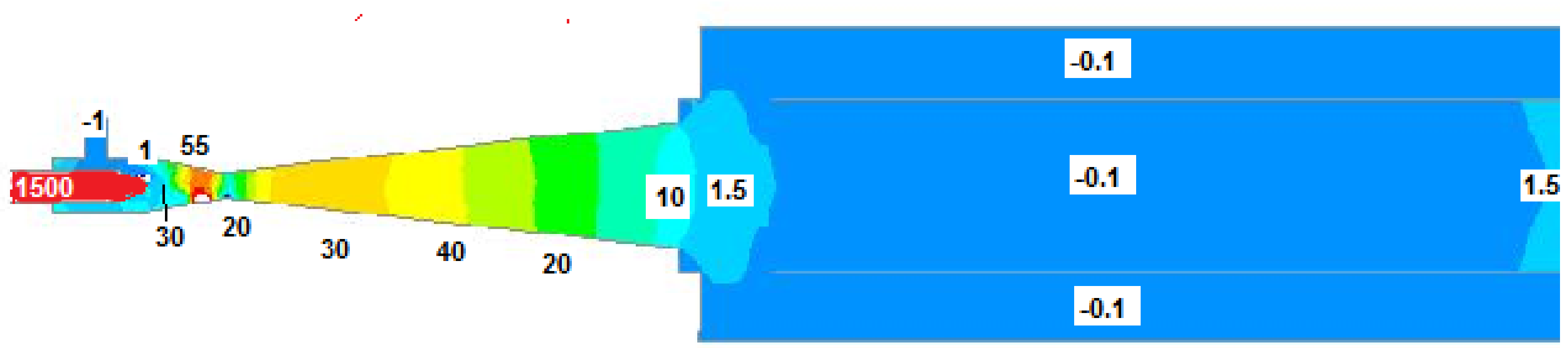
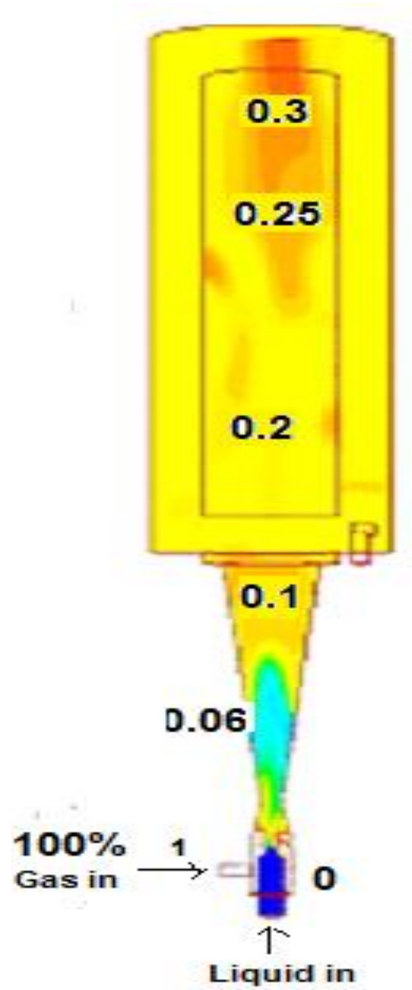
Characteristics of the ejector chamber

Pressure distribution (static pressure, kPa)



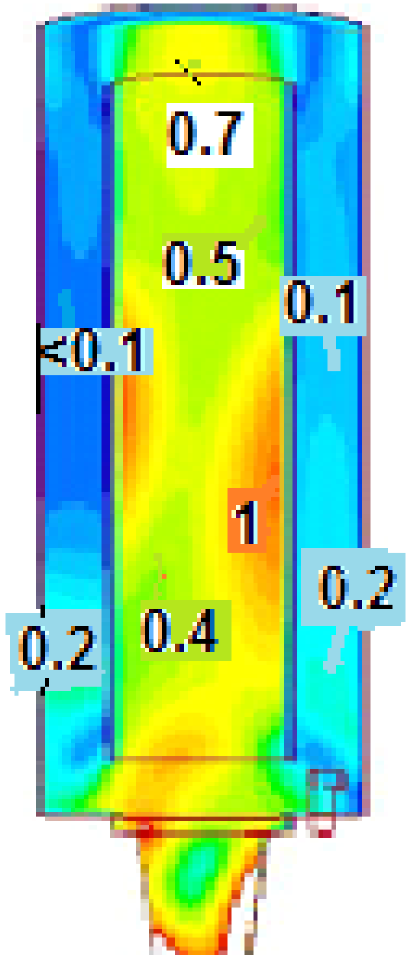
Characteristics of ejector chamber

Phase volume fraction



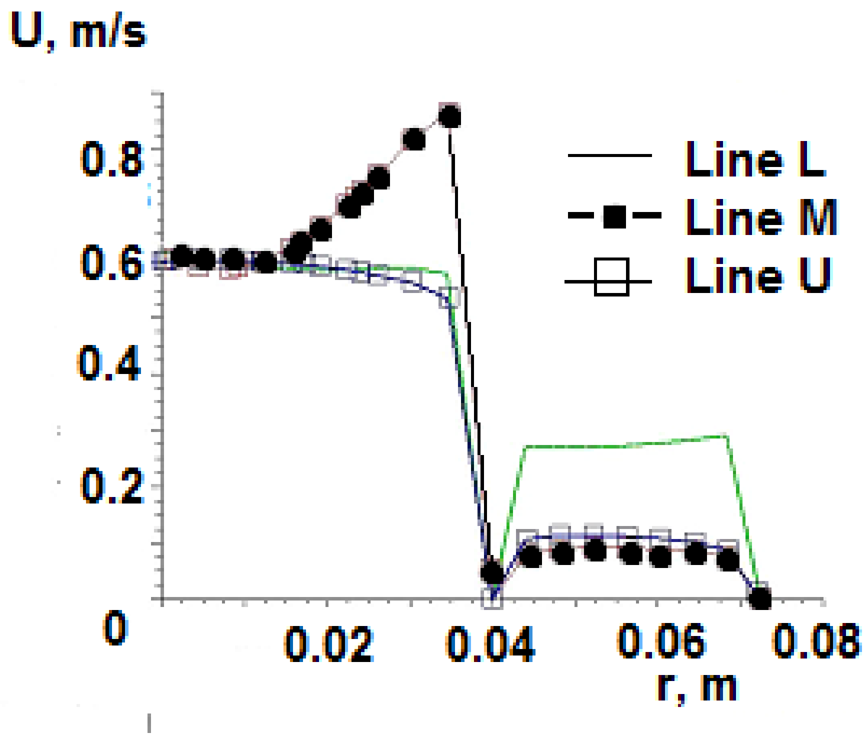
Characteristics of ejector chamber

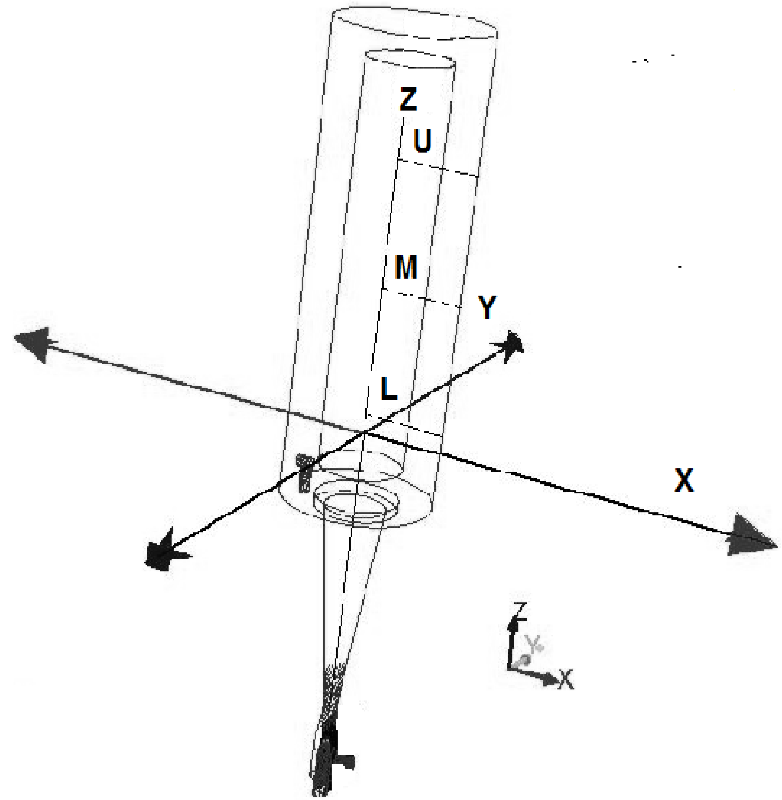
- Velocity (m/s) distribution in air-flow plane



Characteristics of ejector chamber

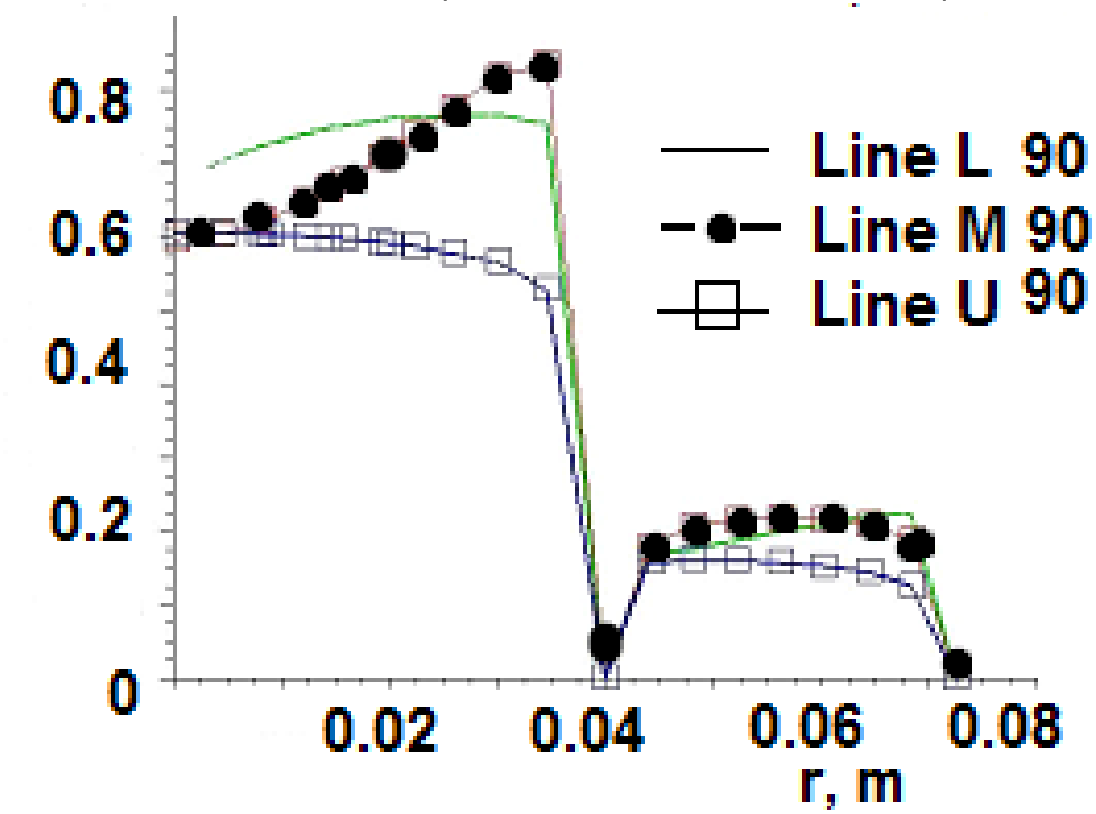
- **Performance close to electrode surface**

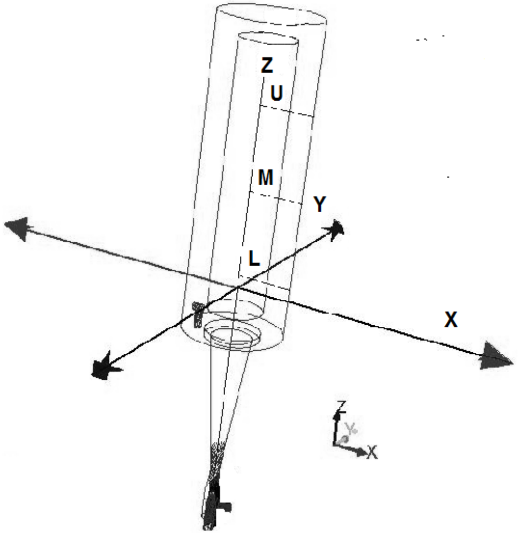




Characteristics of ejector chamber

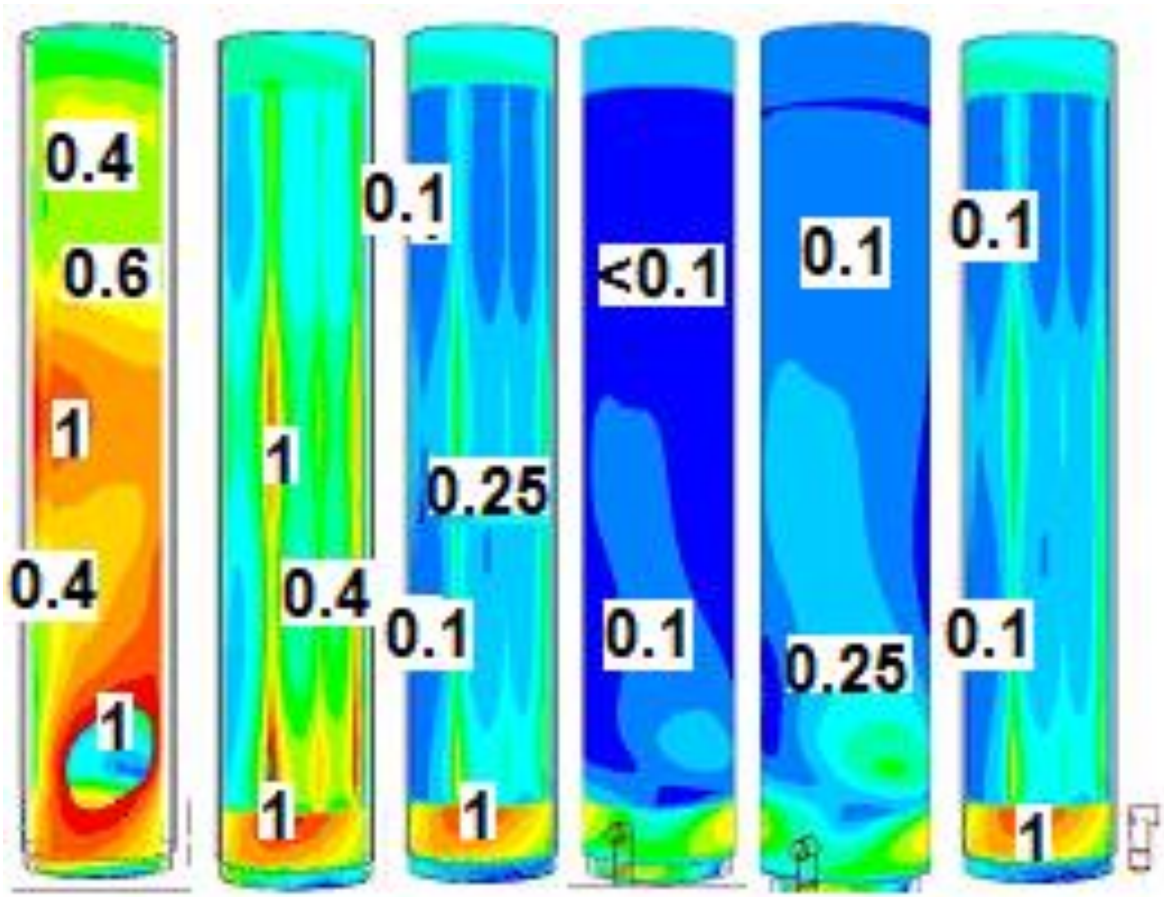
Velocity radial profiles over the electrode surface, e.g. r=0.04m, and near to it (r=0.035m, r=0.045m); r is radial coordinate.”





Characteristics of ejector chamber

Example velocity distribution (in m/s) over the solid-liquid interface (the cathode); radial coordinate **r** varies within the range +/- 5mm).



The framework of further studies:

(1)mesh refinement and
(2) further cell geometry

Mesh Refinement

or

What has been done on the project between the two recent meetings **?**

(1) Mesh 3 was elaborated for a study with increased number of cells from 700000 to 1.1 mln.

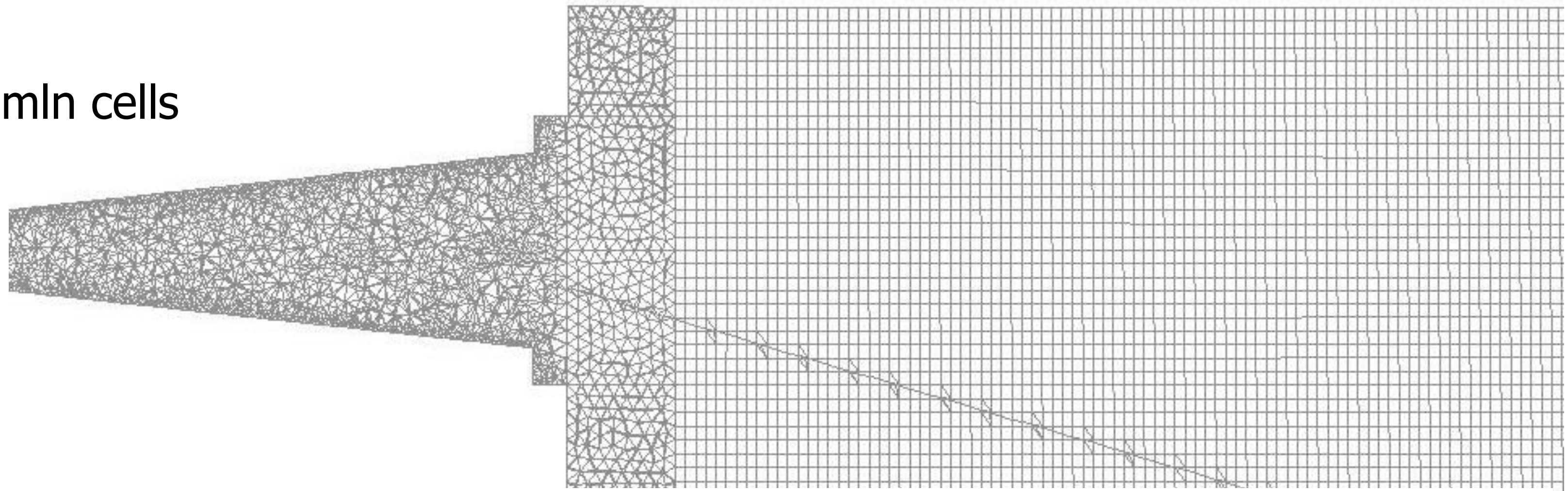
(2) Mesh 4 was elaborated for another study with further increase of the NC from 700 000 to 3.5 mln.

(3) Solutions for these discretizations of the numerical scheme

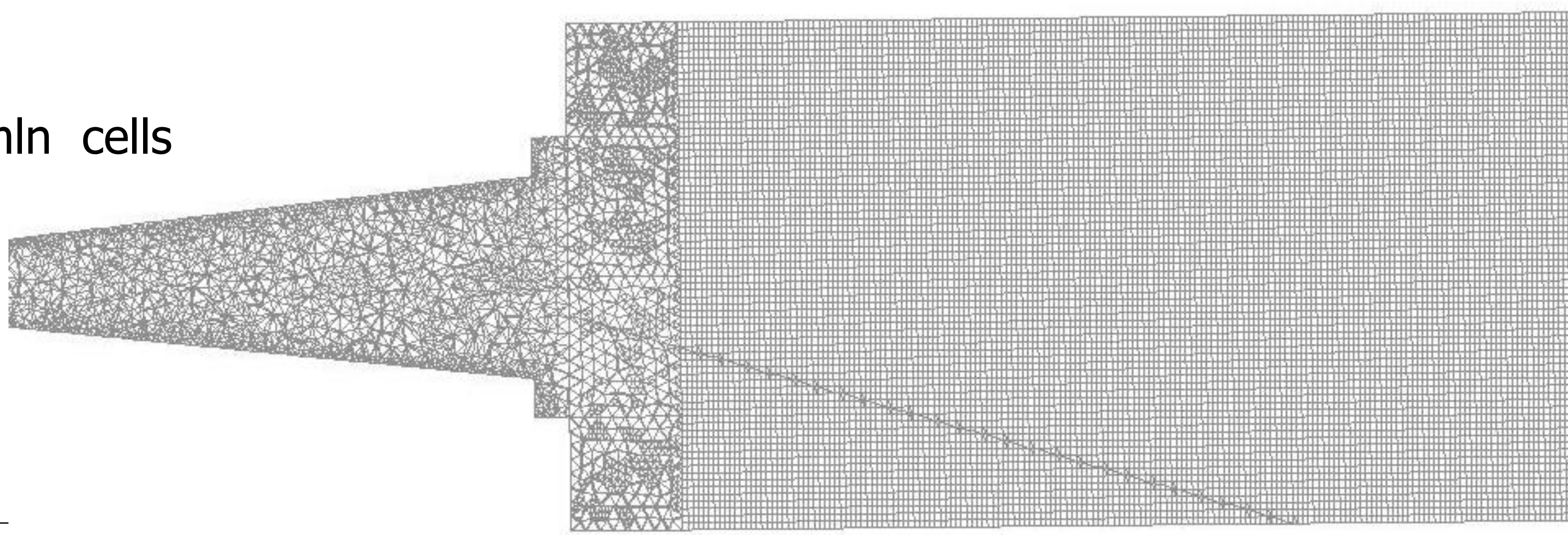
(4) New RESULTS obtained

Mesh refinement

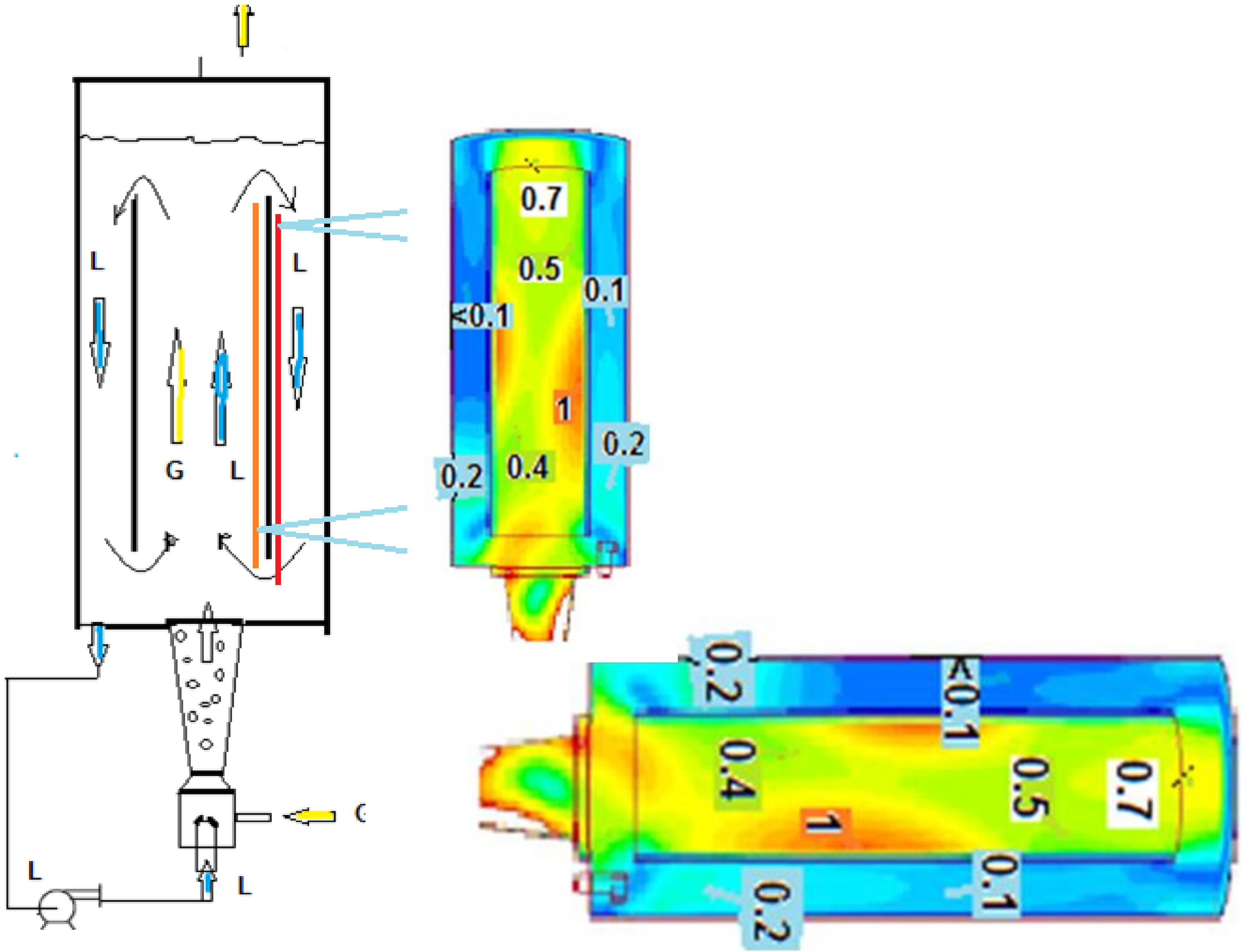
0.14 mln cells



1.1 mln cells

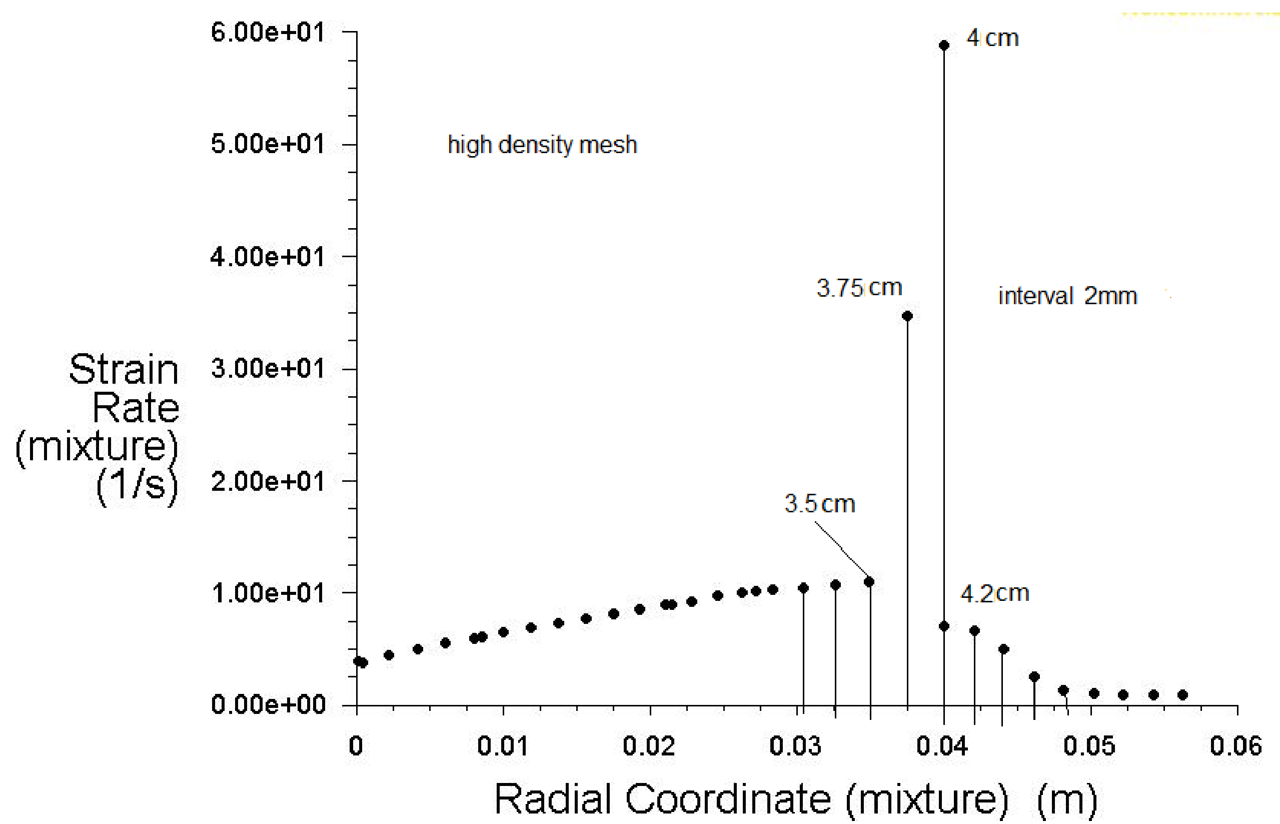


Focus on the cathode active surface



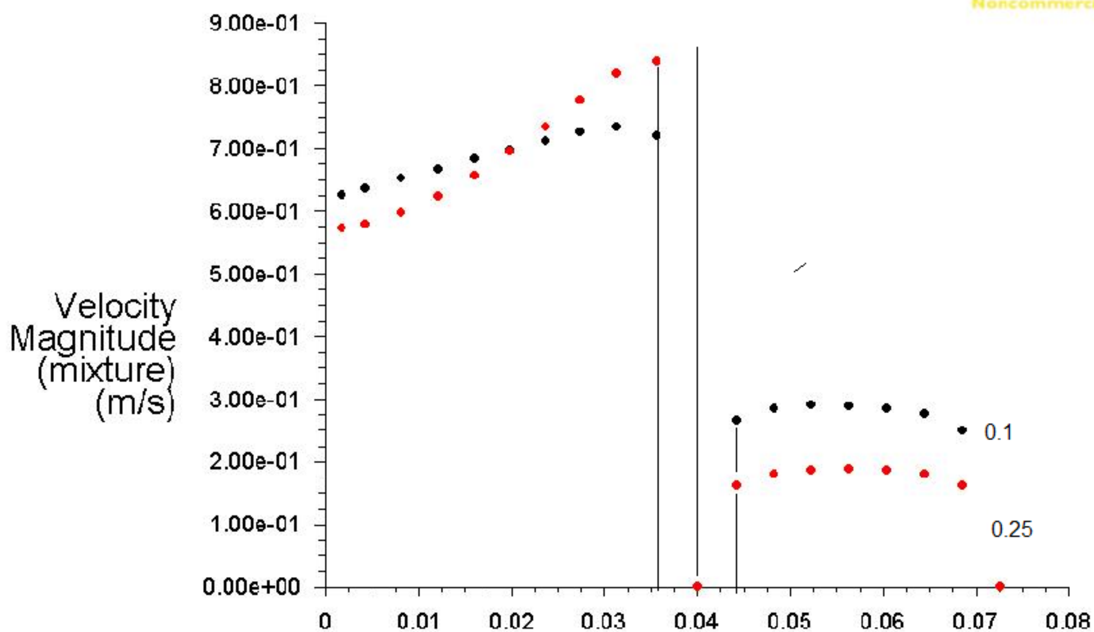
Comparison of mesh refinements 3 and 4

Example with about 1mln cells.

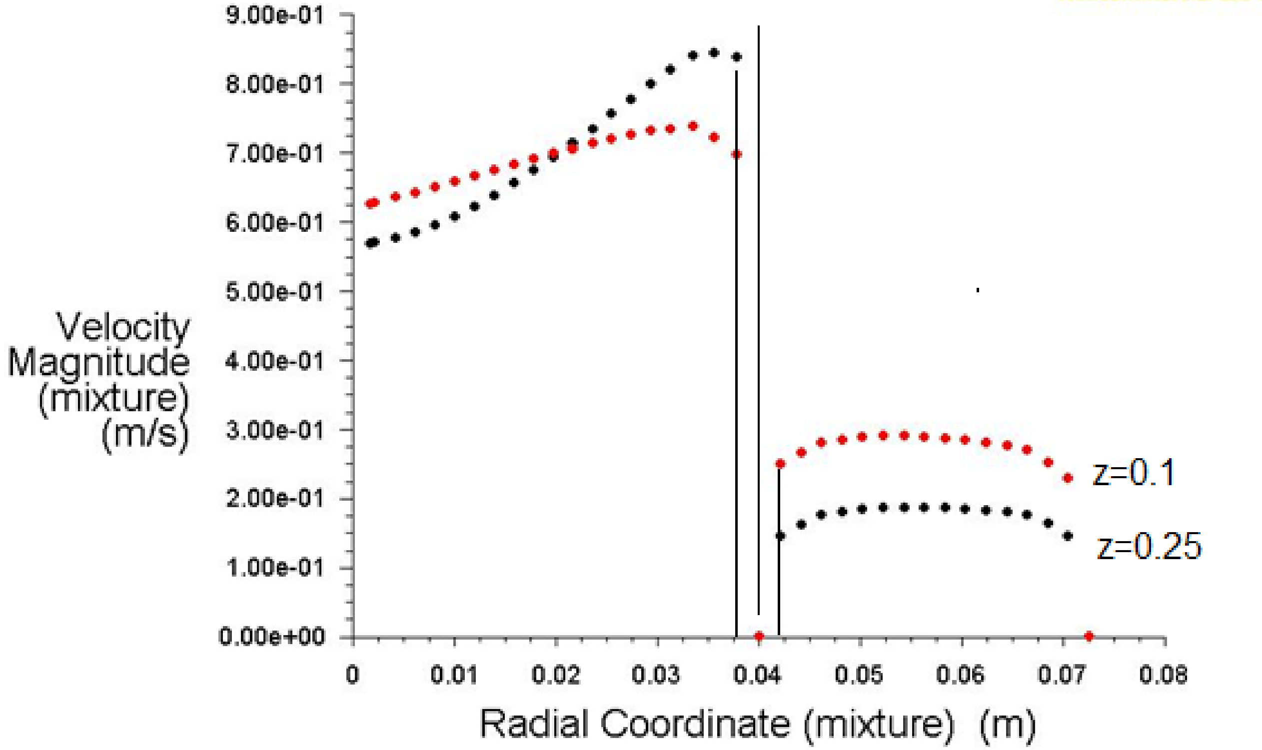


Resolution 2mm allowing enhanced interpolation down to 200 µm.

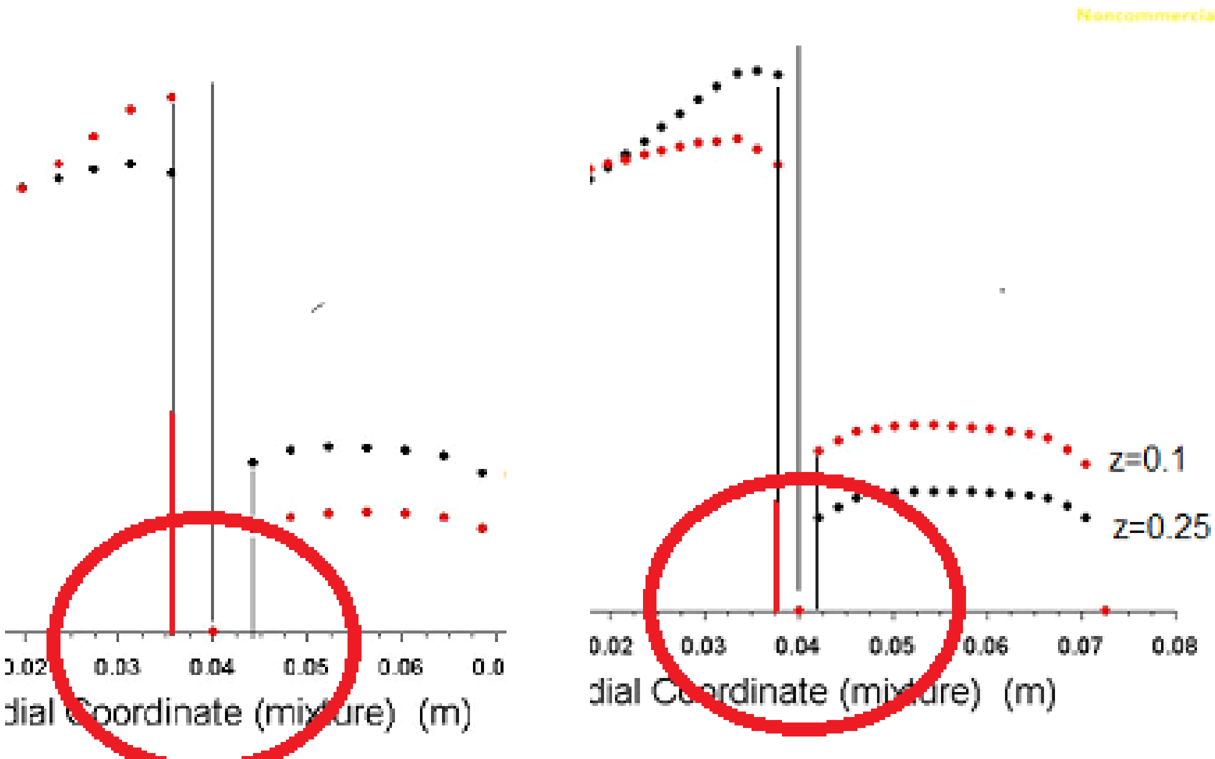
0.1 mln cells



1 mln cells



Comparison of velocities at different cell density

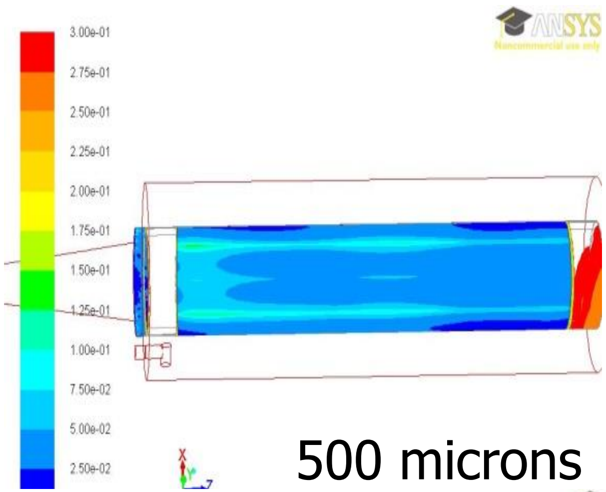


Case of 0.1 mln cells

Case of 1 mln cells

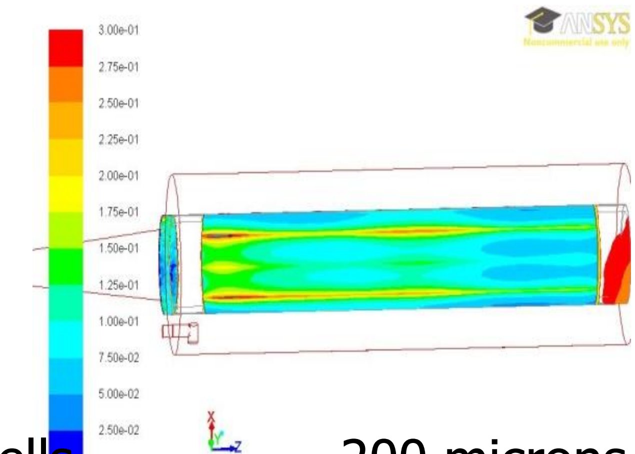
Comparison of velocity contours

0-500 µm off the electrode internal surface

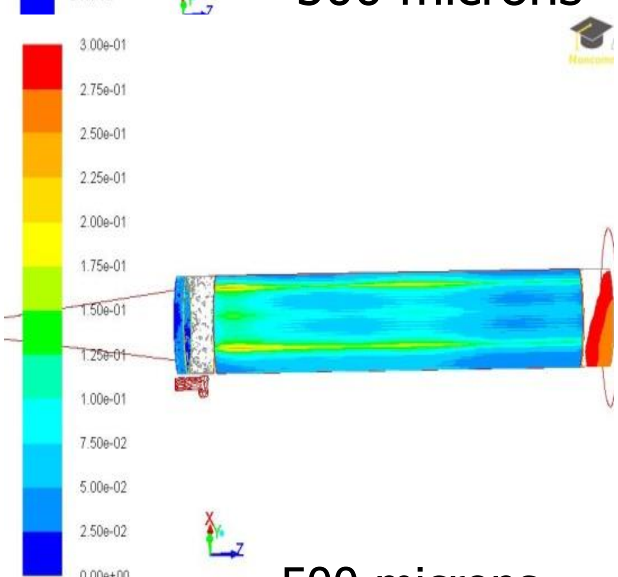


500 microns

0.1 mln cells

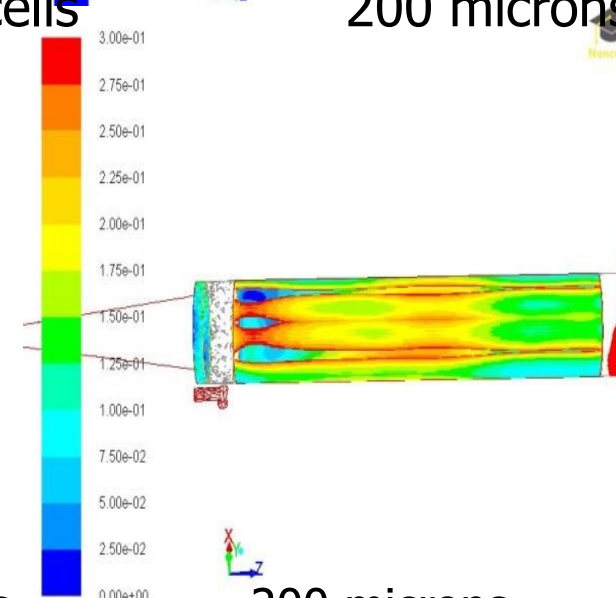


200 microns



500 microns

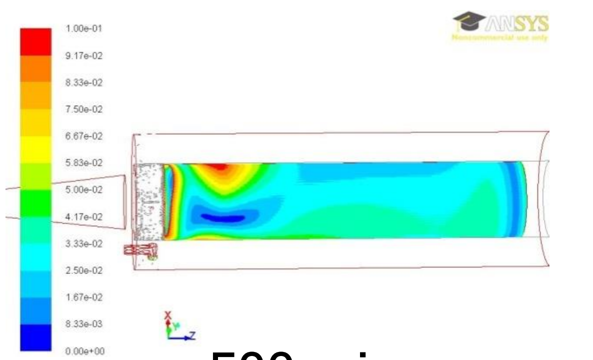
1 mln cells

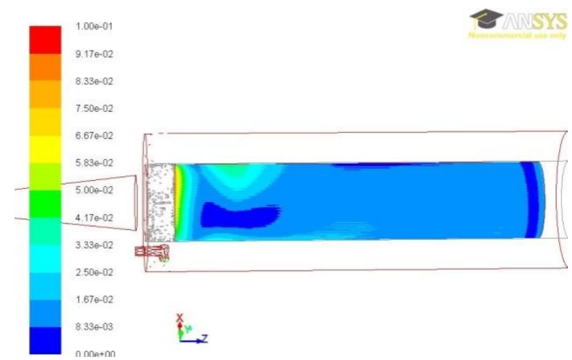


200 microns

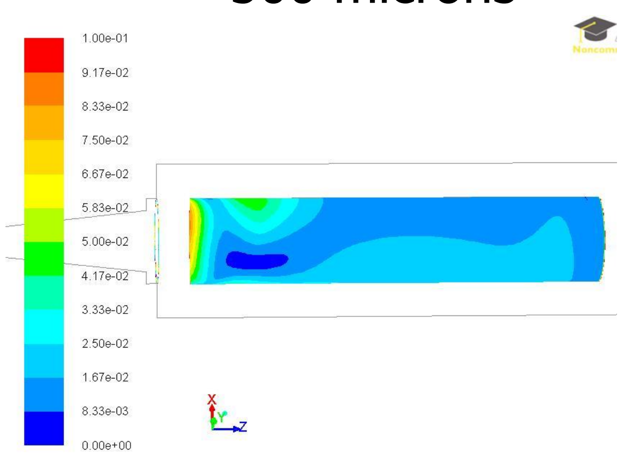
Comparison of velocity contours

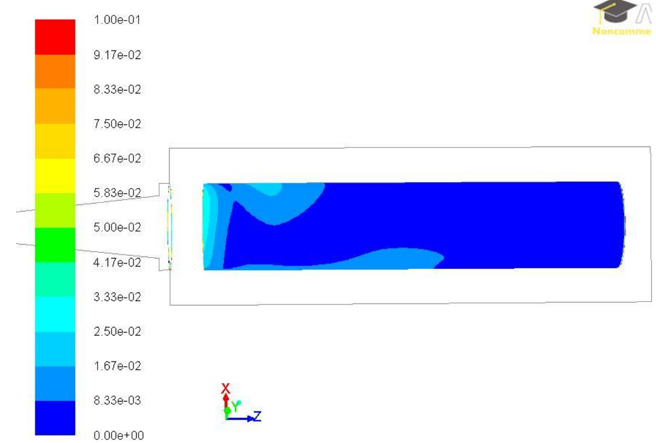
0-500 µm off the electrode external surface





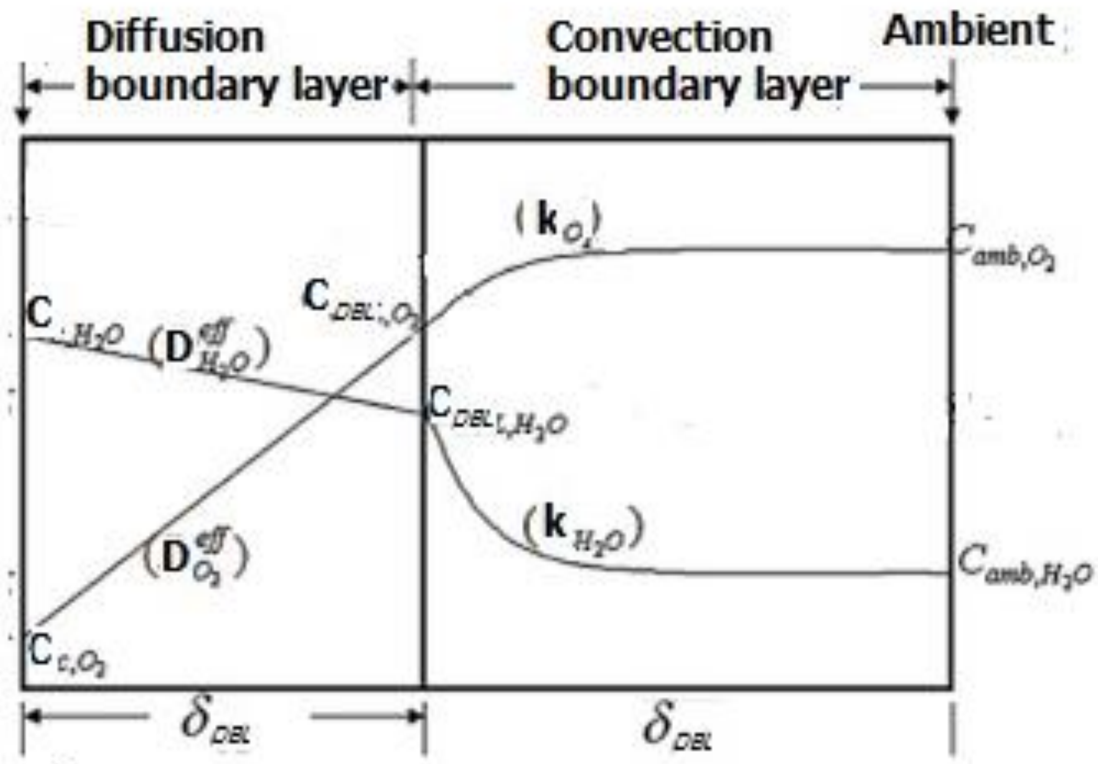
500 microns 1 mln cells 200 microns





500 microns 0.1 mln cells 200 microns

Mass transfer is important



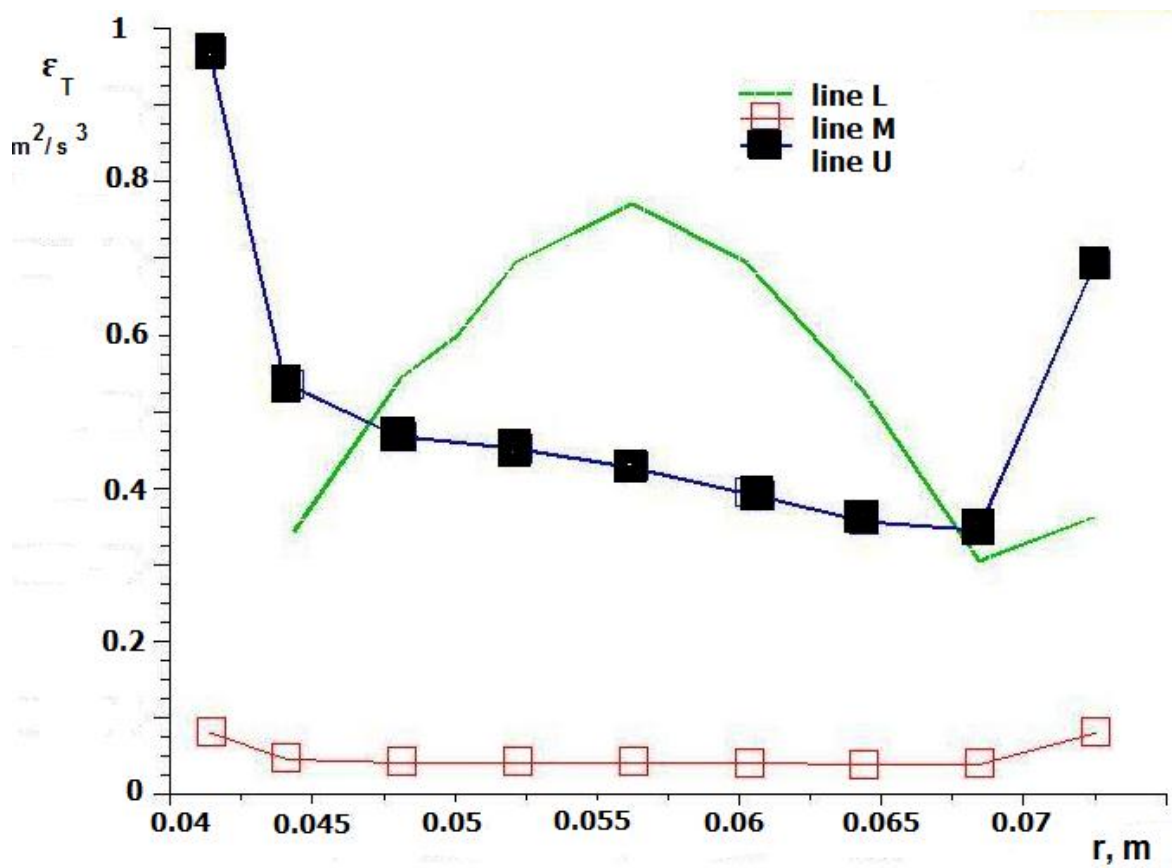
Characteristics of ejector chamber

- Flow radial ϵ_T – as determined by the equation

$$k_L = \frac{2}{\sqrt{\pi}} \sqrt{D_{ab}} \left(\frac{\varepsilon_T \rho_L}{\mu_L} \right)^{1/4}$$

Characteristics of ejector chamber

Flow radial ϵ_T – profile corr. to levels L, M, U



Process evaluation and estimates

- Liquid-phase mass transfer coefficient. (prognostic values)

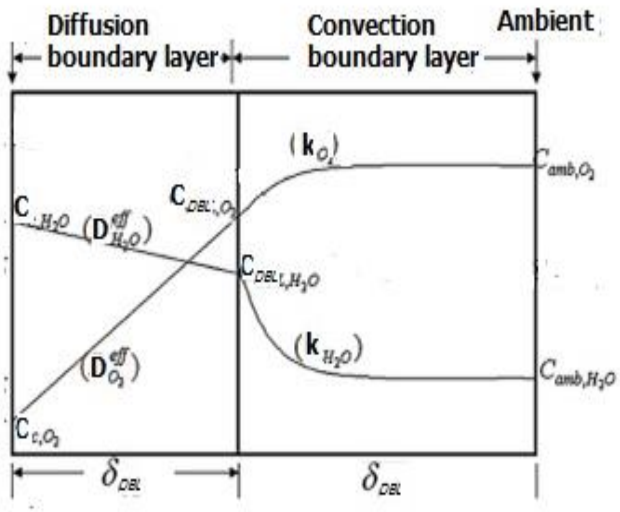
Position eps m^2/s^3	1	0.4	0.04	10	100
k_L, m/s	15.6×10^{-4}	6.24×10^{-4}	0.66×10^{-4}	2.7×10^{-3}	5×10^{-3}

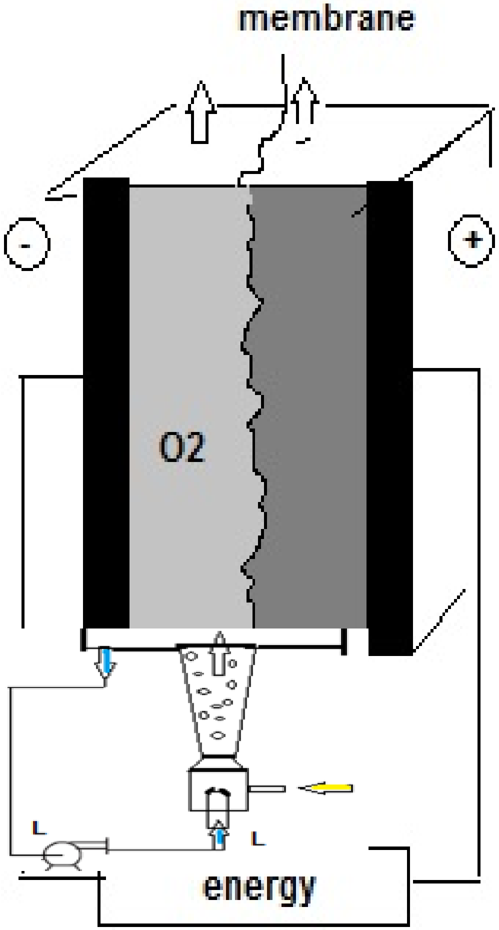
The framework of further studies:

(2) Study another cell geometry

2. The framework of the further study:

solution of further cell geometry
and what is intended to be done



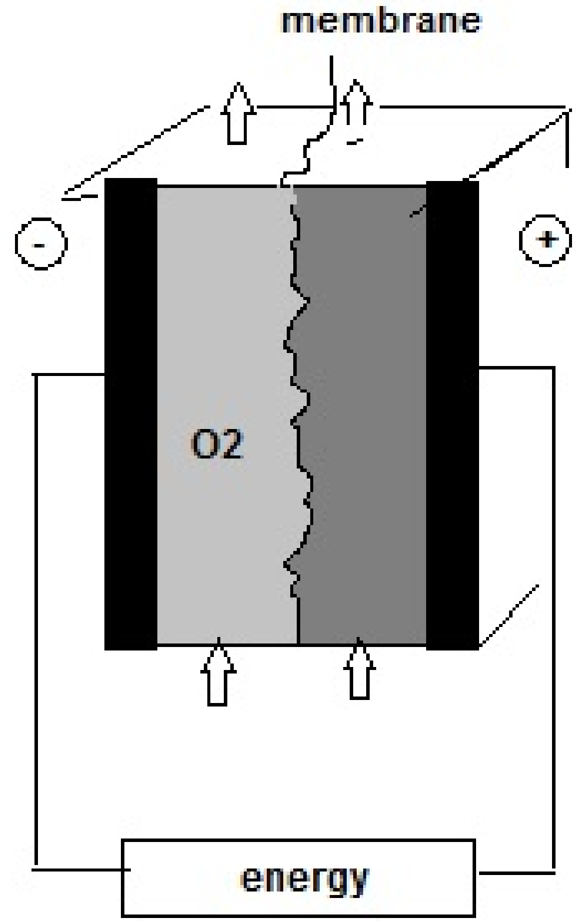


to uncover the basic relationships of the operating variables and cell design

In conclusion

The framework of further studies further cell geometry

Characterization of a fuel cell (FC) cathode chamber (equipped) with ejector mixer in view of (focused on) intensification of the oxygen reduction reaction (ORR).



Further work

- Further work is needed to uncover the basic relationships of the operating variables and cell design, namely, liquid flow rate and nozzle geometry, as well as the geometry of the cell cross section, e.g. cylindrical or rectangular.
- Essentially, the model in its present form can be combined with the current distribution model (Ohm's law for ionic conduction), the electrode kinetic expressions (Butler-Volmer) and a diffusion convection equation for the ionic transport and be implemented for complete description of current distribution and cell voltage thus promoting future analyses of the energy-storage system

Acknowledgement

The study is supplement to Project HYSULFCEL, supported by [BS-ERA.NET](BS-ERA.NET)

Thank you!

Important references

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