Application of COMSOL Multiphysics in the Simulation of Magnesium (Mg) Refining and Production

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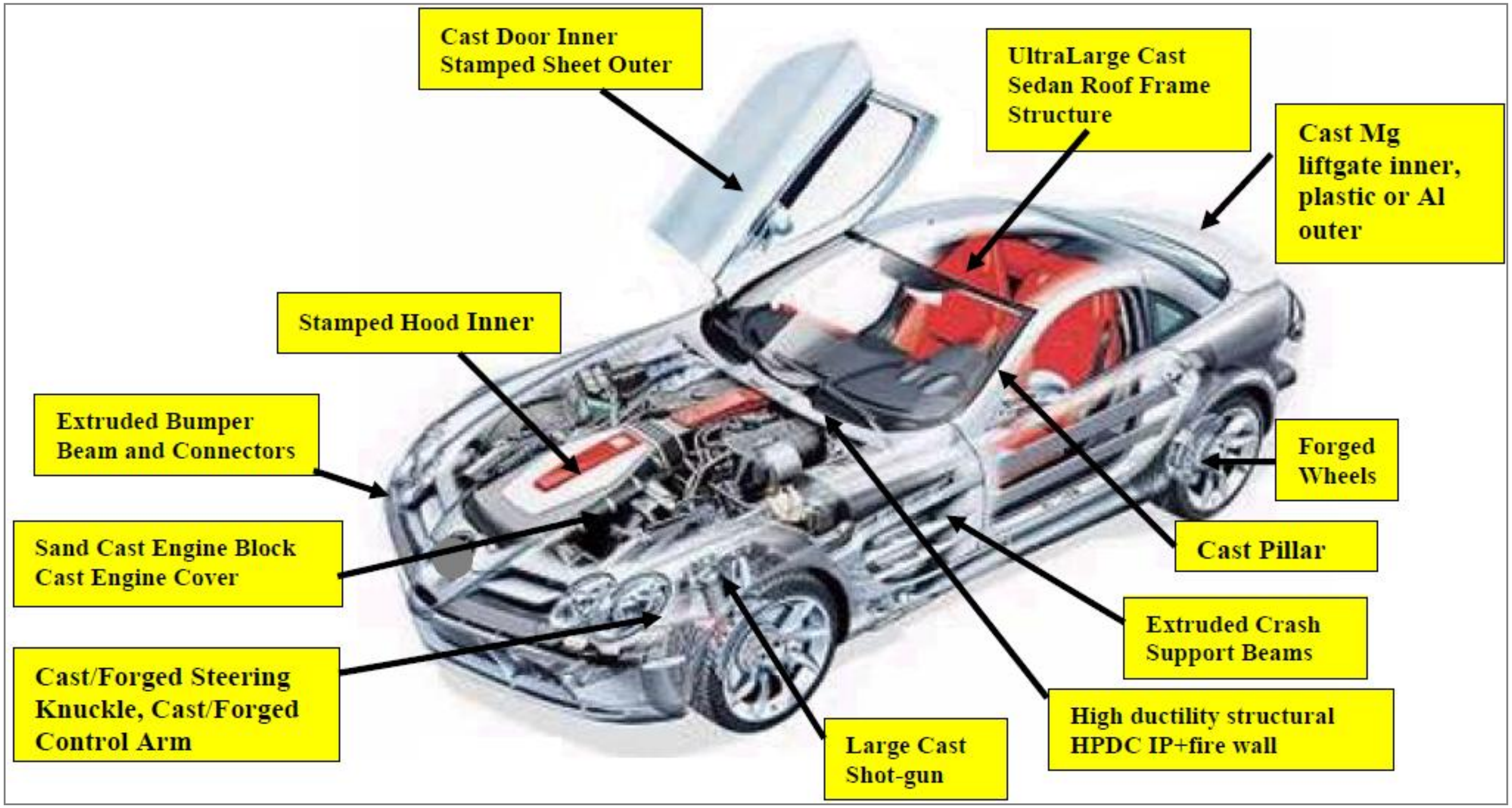
Outline

- Introduction
- Magnesium refining process
    - Modeling the refining process
    - Conclusions
- Magnesium electrolysis process
    - Modeling the flow behavior in the flux
    - Conclusions

Introduction

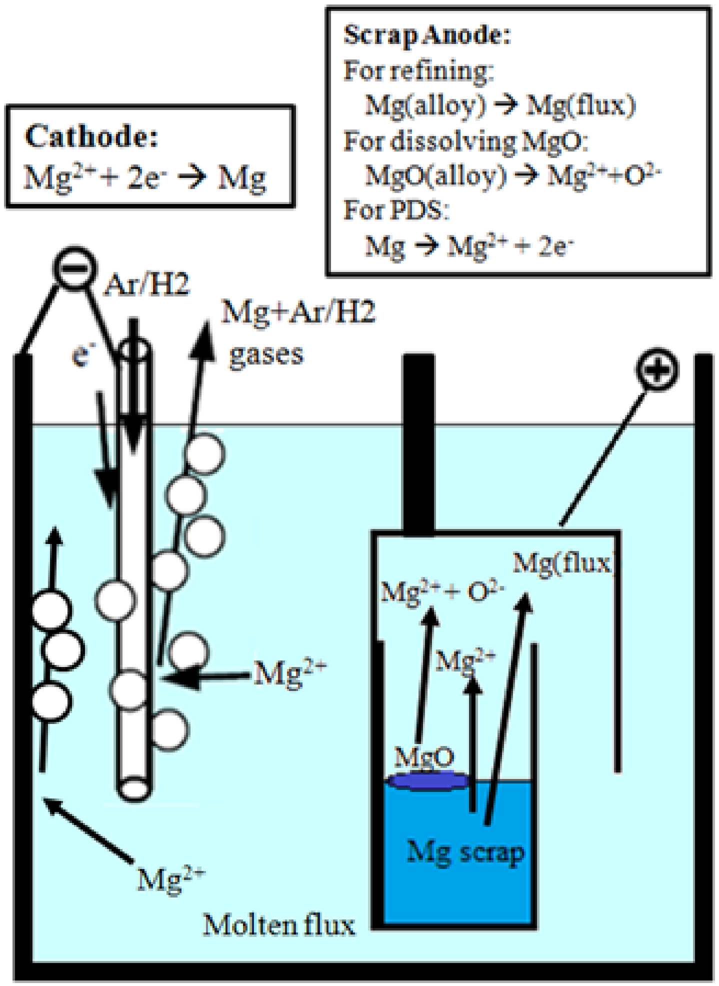
- Advantages of Mg for light-weight vehicles
  - Least dense engineering metal
  - Excellent stiffness-to-weight ratio
  - Low manufacturing costs
- U.S. auto makers would like to replace 630lb of steel and aluminum parts per vehicle with 340lb of Mg alloy by the year 2020[1].

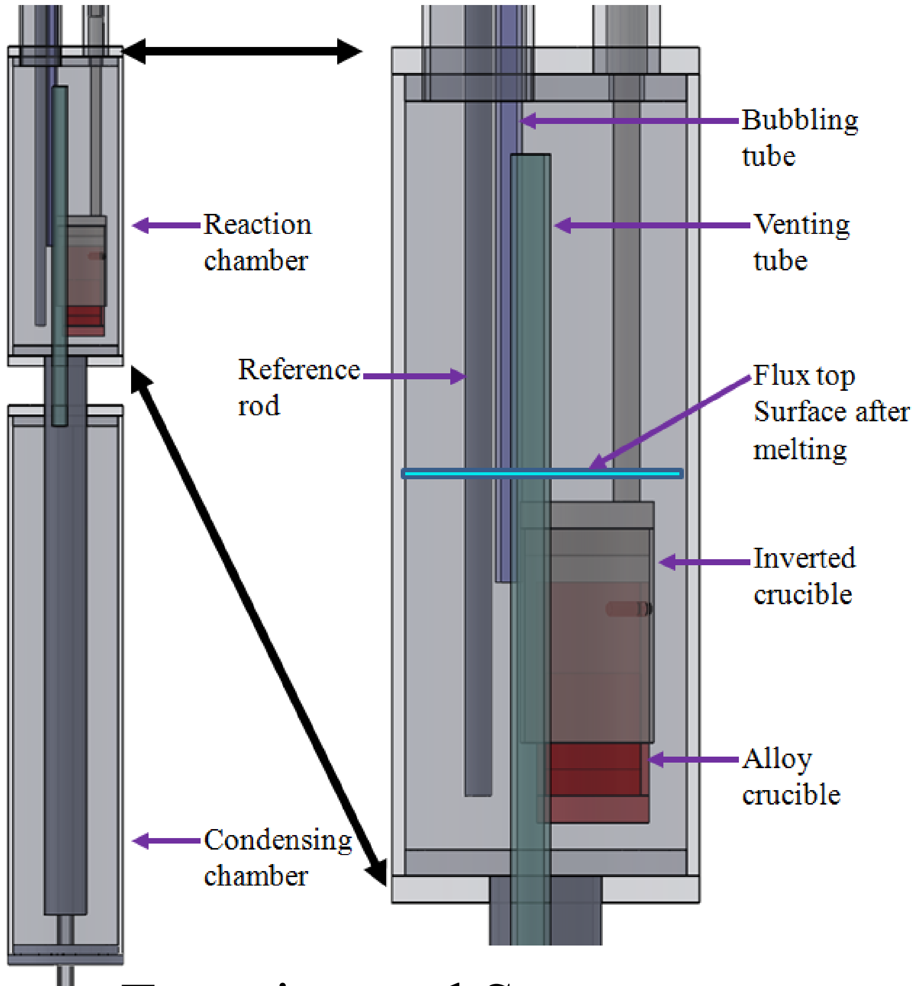


[1]. United States Automotive Materials Partnership (USAMP), Magnesium Vision 2020: A North American Automotive Strategic Vision for Magnesium, Technical Report, USCAR, November 2006.

Process for magnesium refining

- Refine pure magnesium from partially oxidized magnesium scrap alloy by
  - dissolving magnesium and its oxide from scrap into a molten flux, followed by
  - vapor phase removal of dissolved magnesium.

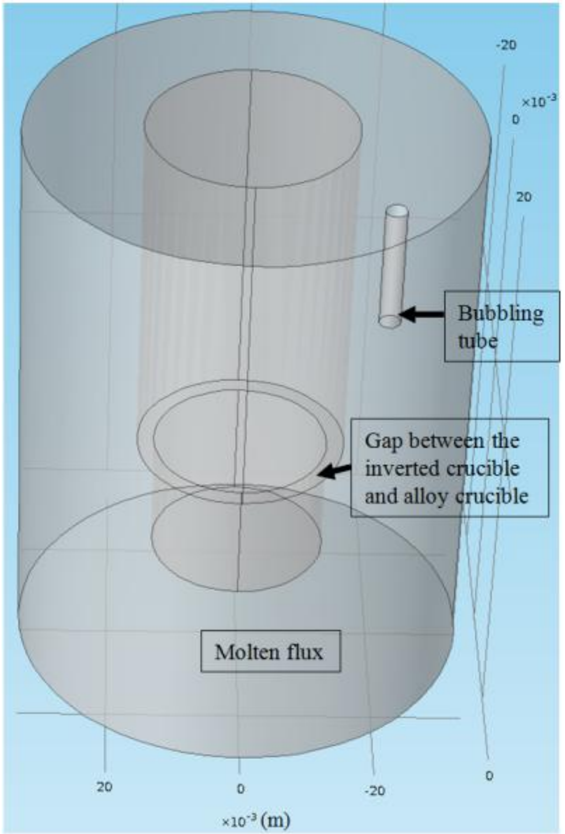




Experimental Setup

Modeling the refining process

- Illustrate the flux flow behavior and Mg transport during argon bubbling
- Assumptions
  - Constant temperature, flux density and viscosity
  - Wall thickness of the bubbling tube is neglected.
  - Argon bubble size is half of the inner diameter of the bubbling tube.



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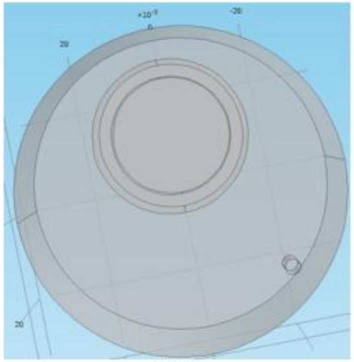
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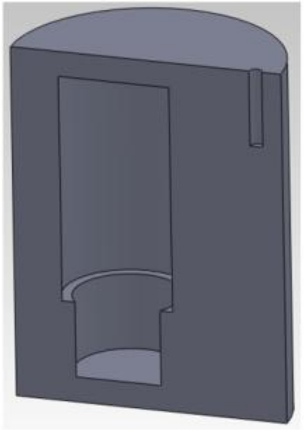

(c)

- Modeling
  - COMSOL Multiphysics 4.2a
    - Laminar bubbly flow mode
    - Transport of diluted species mode
  - Momentum transport equation

$$\phi_l \rho_l \frac{\partial \vec{u}_l}{\partial t} + \phi_l \rho_l \vec{u}_l \cdot \nabla \vec{u}_l =$$

$$-\nabla p + \nabla \cdot \left[\phi_l \eta_l \left(\nabla \vec{u}_l + \nabla \vec{u}_l^{\,T} \right) \right] + \phi_l \rho_l \vec{g}$$

  - Mass transport equation

$$\frac{\partial C_{Mg}}{\partial t} + \nabla \left(-D_{Mg} \nabla C_{Mg} \right) + \vec{u}_l \cdot \nabla C_{Mg} = R_{Mg}$$

$$R_{Mg} = -kC_{Mg}\phi_g = -kC_{Mg}(1-\phi_l)$$

Boundary conditions

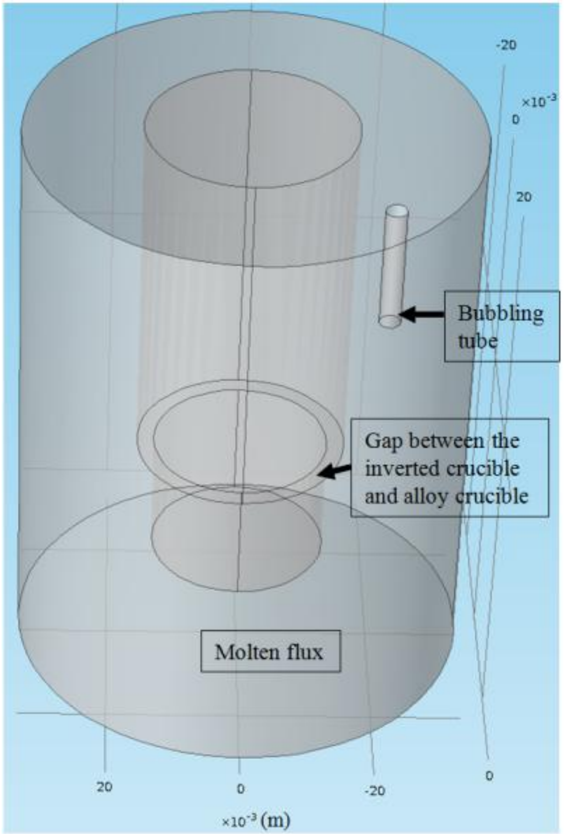
- Laminar bubbly flow mode
  - The bubbling tube bottom is the argon inlet (20cc/min); no liquid slip.
  - The top surface of the molten flux is the outlet of argon; liquid slip.
  - The pressure at the top surface is 1 atm.
  - No gas flow or liquid slip at the remaining walls.
- Transport of diluted species mode
  - The gap is the inlet of Mg (224.57 mol/m^3).
  - At the top surface, the magnesium concentration is set to zero.
  - No magnesium flux at the remaining walls.

Computing

- Transient mode

Initial conditions

- Laminar bubbly flow mode
  - The initial molten flux velocity field is zero.
- Transport of diluted species mode
  - The velocity field used is from the results of the laminar bubbly flow mode.
  - The initial Mg concentration is zero.



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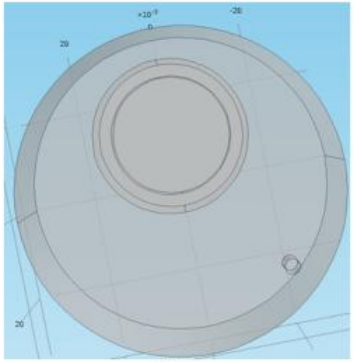
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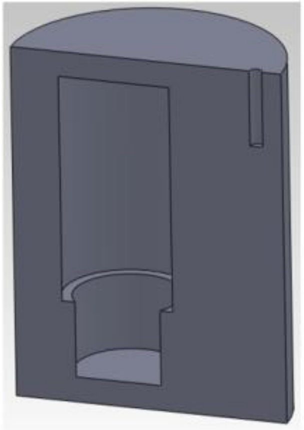
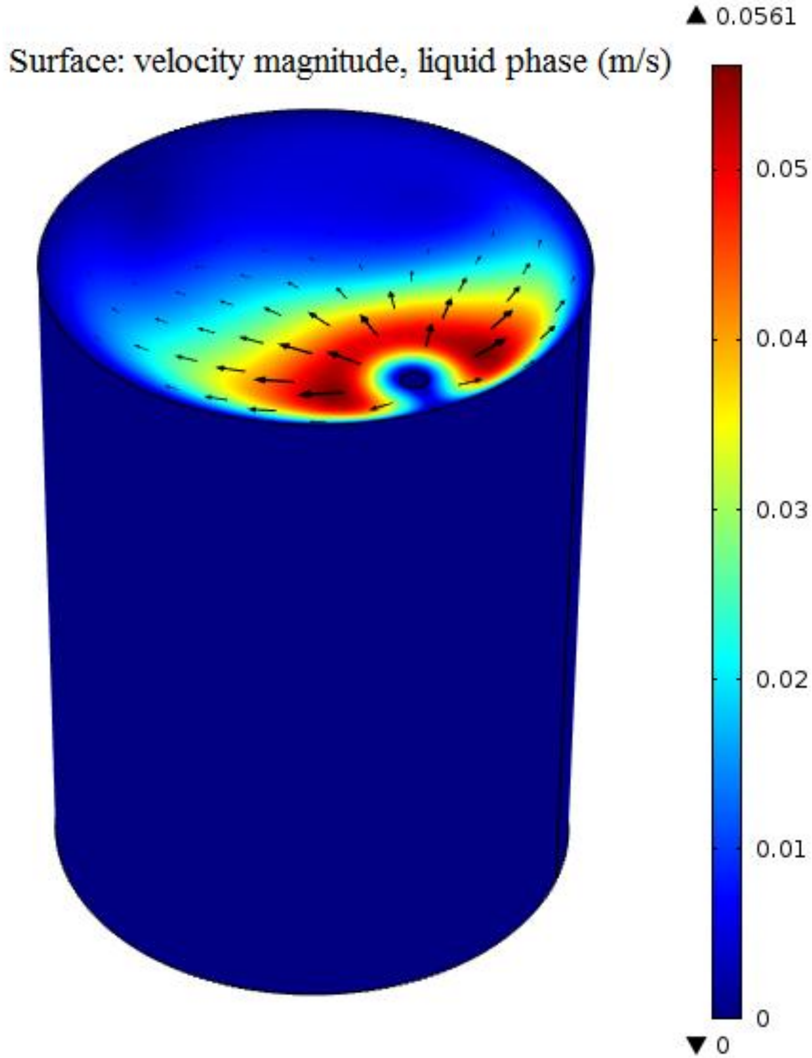
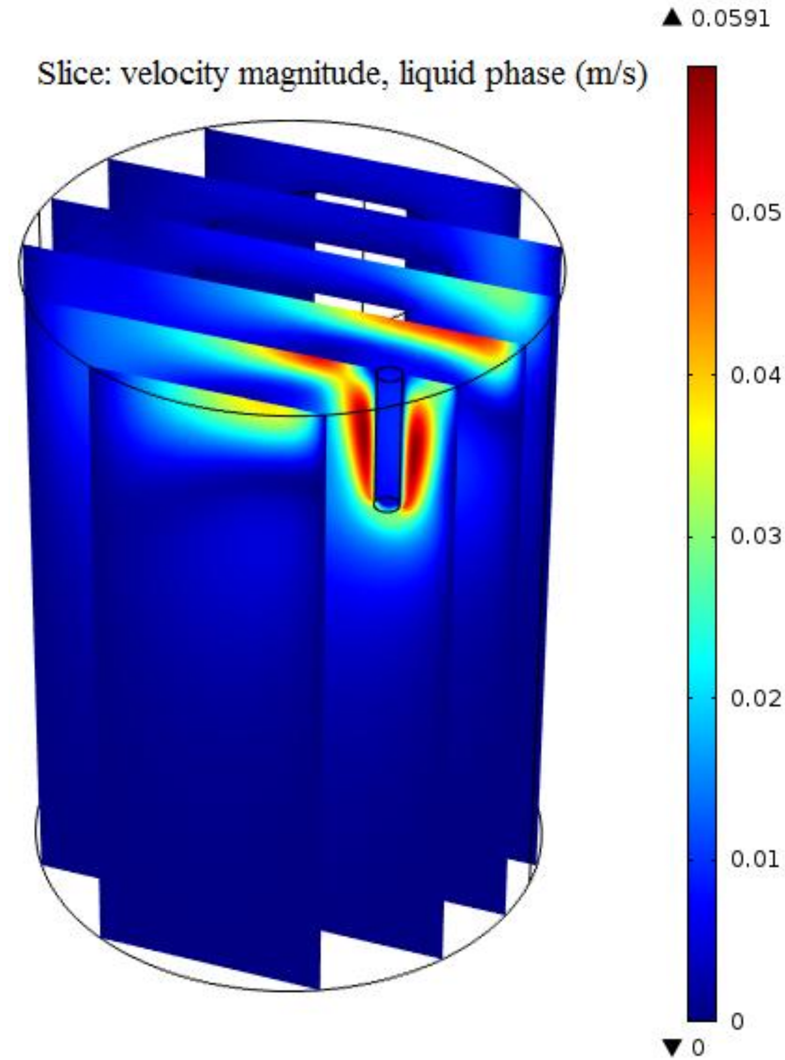
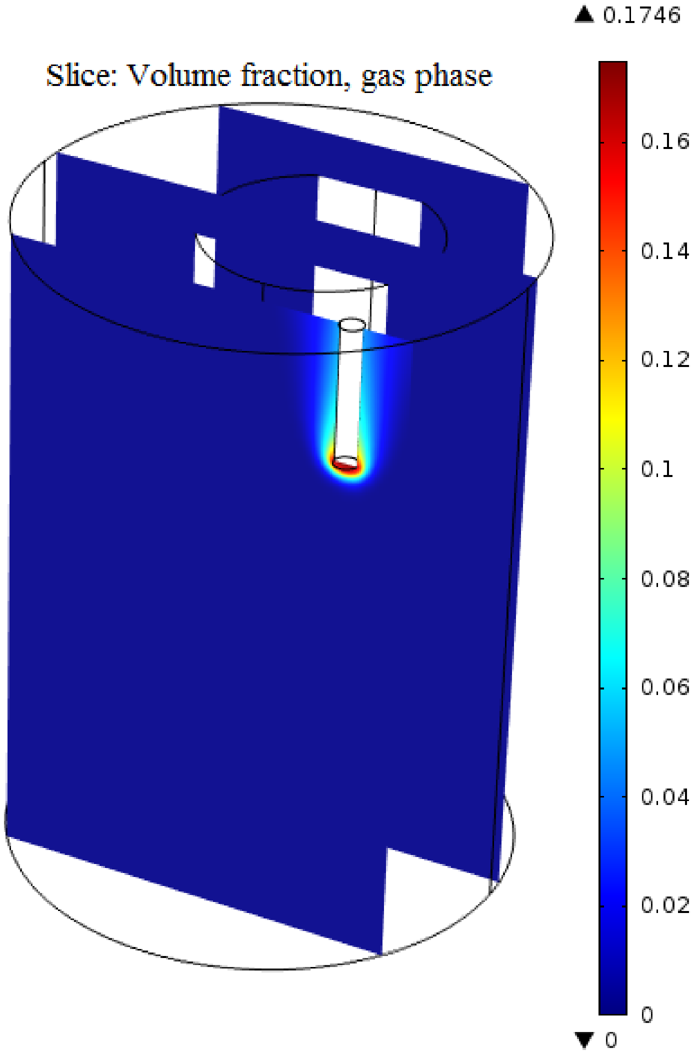

(c)

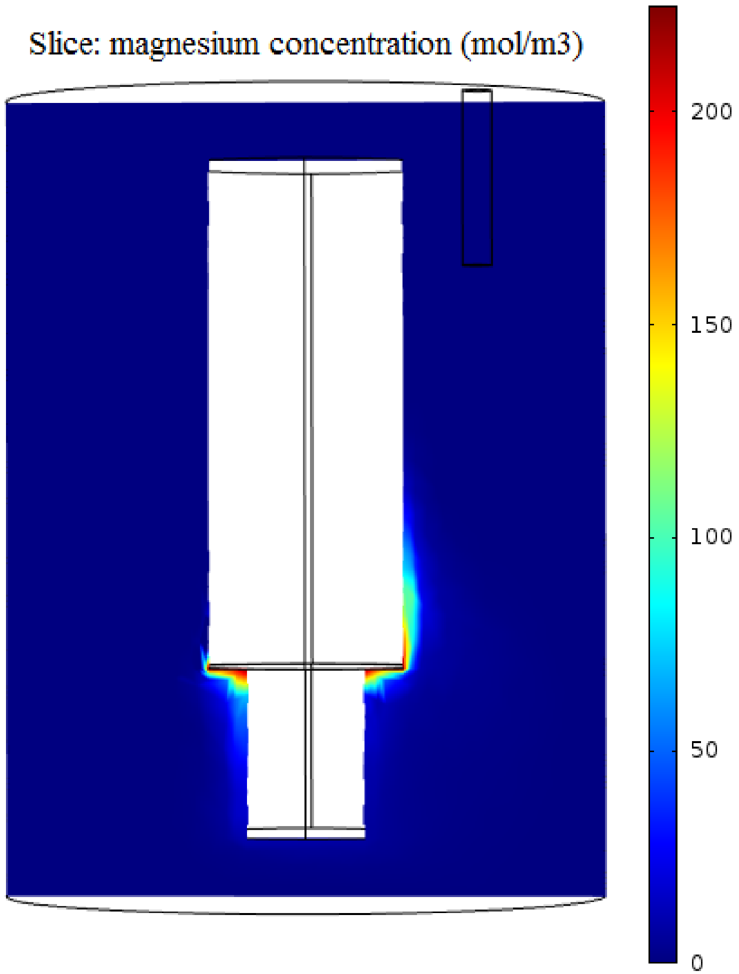
Flow behavior of the flux bubbled with argon (20cc/min)





Volume fraction of argon and magnesium concentration





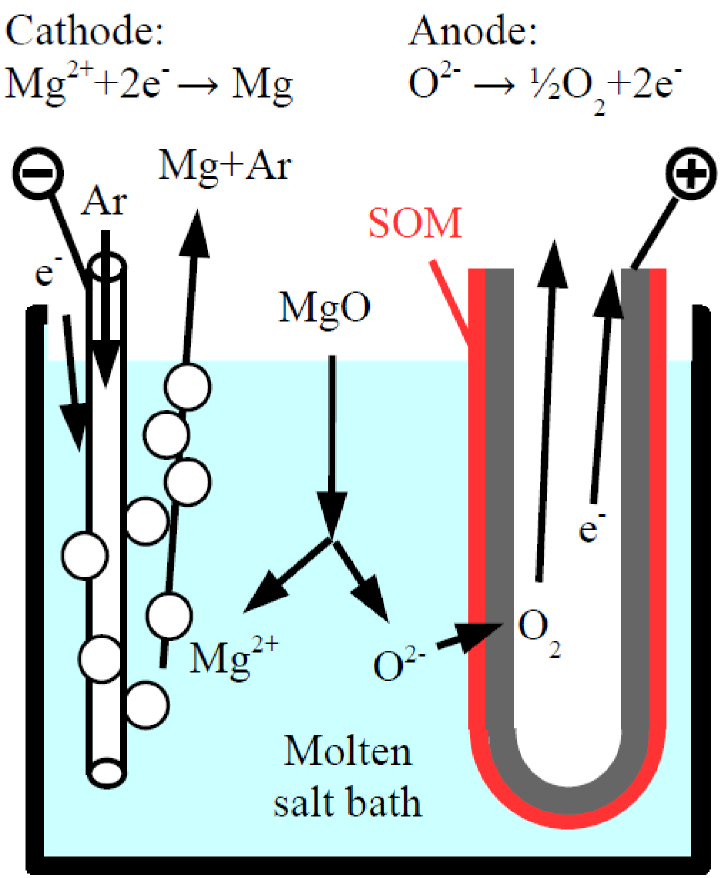
Conclusions

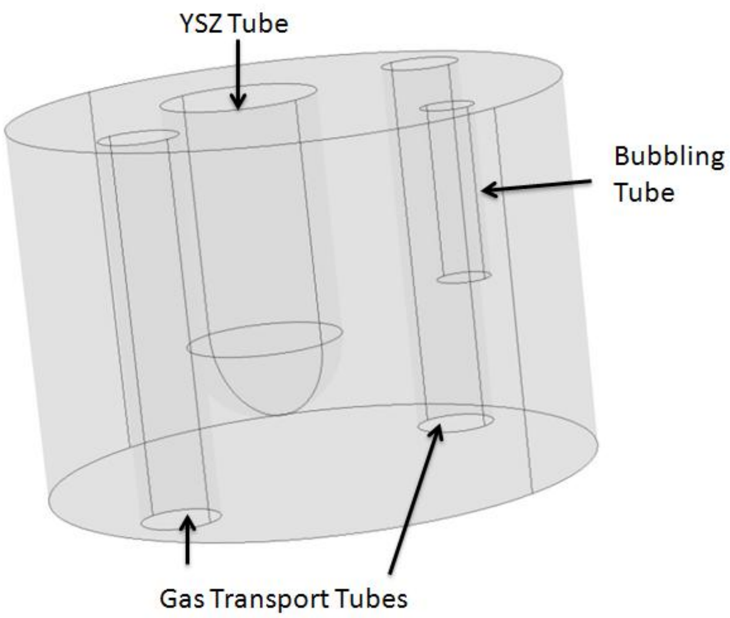
- The modeling successfully simulates and predicts the flow behavior of the molten flux and the magnesium transport during refining.

- It was observed that at the bottom of the of the flux there was a dead zone in which the flux was stagnant.

- Immersing the stirring tube deeper into the flux or increasing the stirring rate can increase the refining rate.

Process for magnesium electrolysis





Modeling the flow behavior during electrolysis

- Illustrate the flow behavior of the flux bubbled with argon during electrolysis at various pressures.
- Assumptions
  - Constant temperature, flux density and viscosity
  - The wall thickness of the bubbling tube is neglected.
  - The argon bubble size is half of the inner diameter of the bubbling tube at 1atm.
  - Under reduced pressures, the bubble diameters was calculated according to the ideal gas law.

$$\left.\begin{aligned} P_i V &= nRT \\ V &= \frac{\pi d^3}{6} \end{aligned}\right\} \Rightarrow d = \left(\frac{6nRT}{\pi P_i}\right)^{\frac{1}{3}}$$

Pressure (atm)	Bubble diameter (mm)
1	1.5875
0.8	1.7100
0.6	1.8822
0.4	2.1546

Modeling of the flow behavior of flux during electrolysis

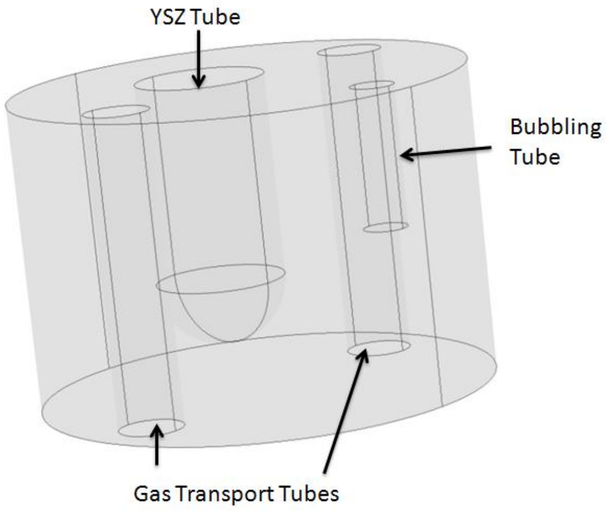
- Modeling
  - COMSOL Multiphysics 3.5a
    - Laminar bubbly flow mode
  - Momentum transport equation

$$\phi_l \rho_l \frac{\partial \vec{u}_l}{\partial t} + \phi_l \rho_l \vec{u}_l \cdot \nabla \vec{u}_l =$$
$$-\nabla p + \nabla \cdot \left[\phi_l \eta_l \left(\nabla \vec{u}_l + \nabla \vec{u}_l^{\,T} \right) \right] + \phi_l \rho_l \vec{g}$$

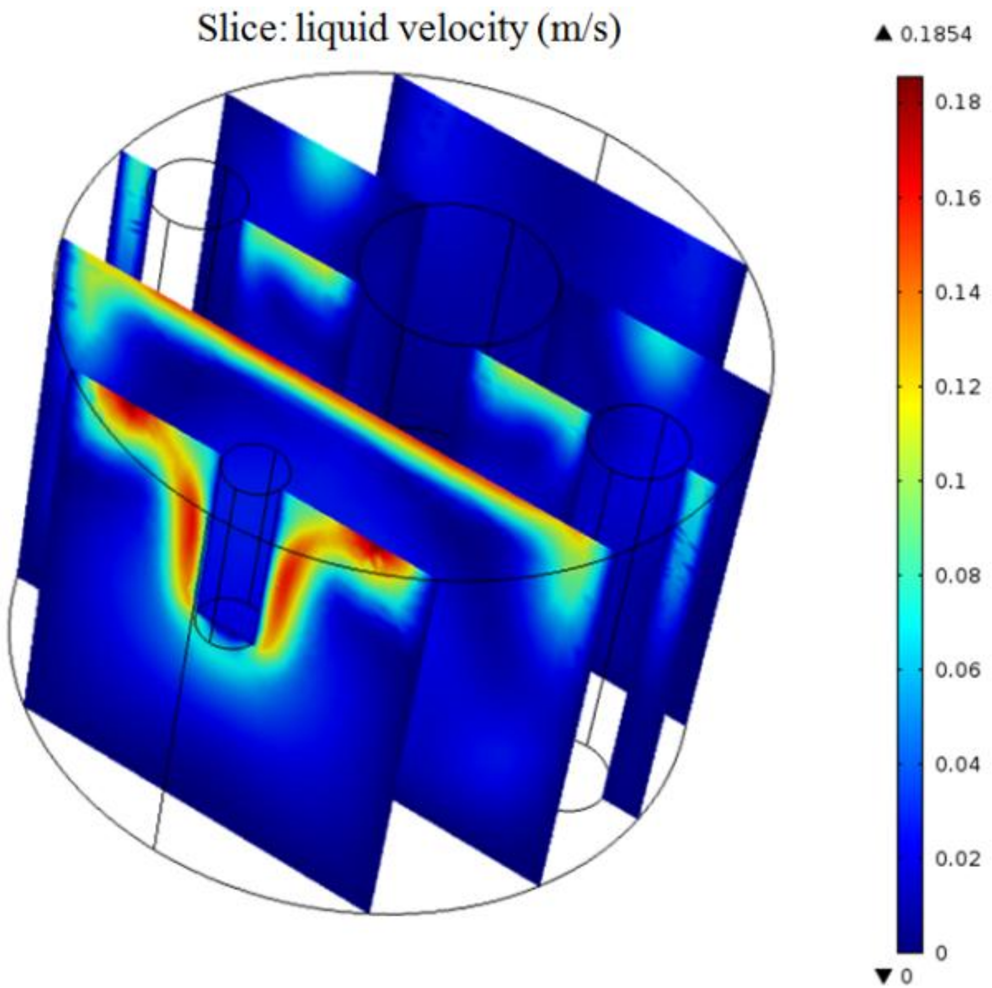
- Boundary Conditions
  - Laminar bubbly flow mode
    - The bubbling tube bottom is the argon inlet; no liquid slip.
    - The top surface is the argon outlet; liquid slip.
    - The pressure at the top surface of the molten flux is set to different values.
    - No gas flow or liquid slip at the remaining walls.

- Initial condition
  - The initial molten flux velocity is zero.

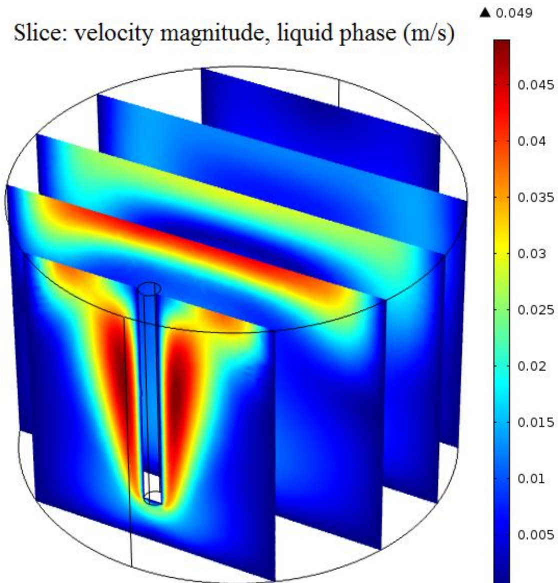
- Computing
  - Transient mode



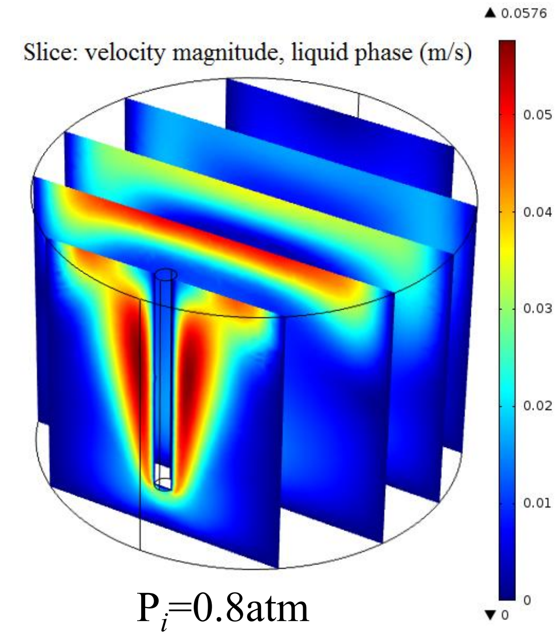
Flow behavior of the flux bubbled with argon (100 cc/min)



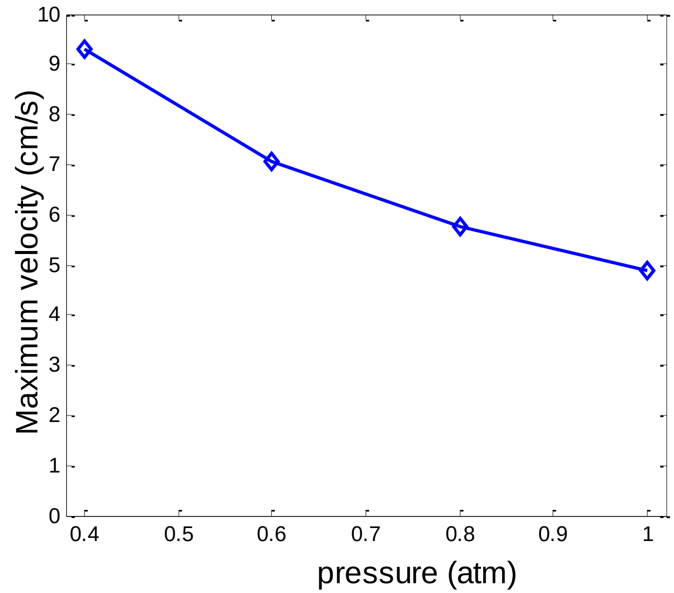
Flow behavior of the flux under reduced pressures (15cc/min)

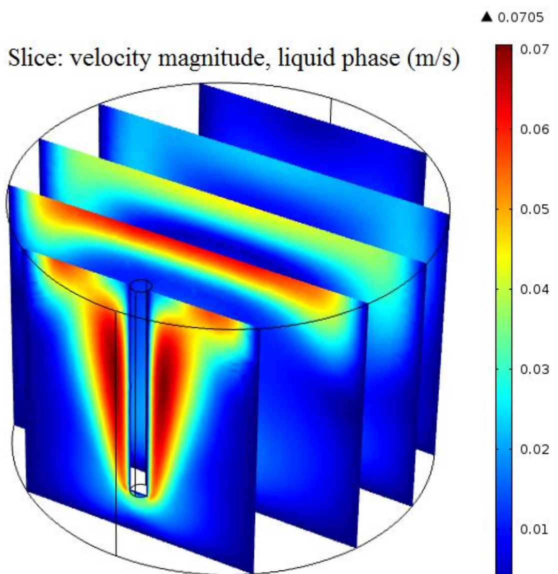


P_i=1atm

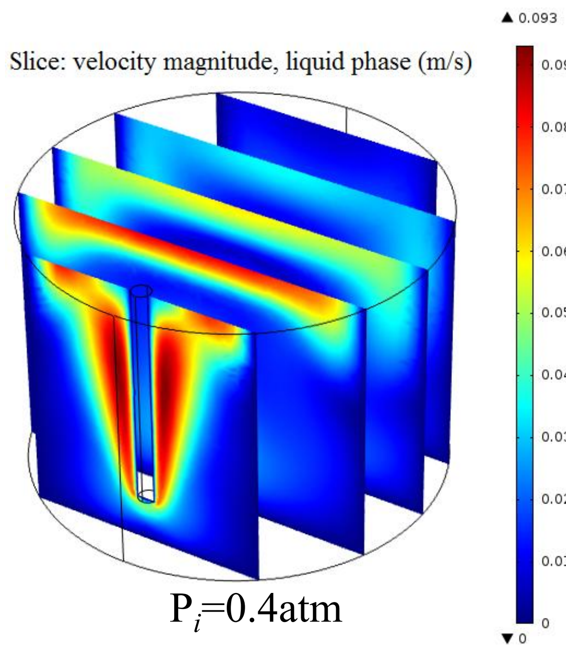


P_i=0.8atm

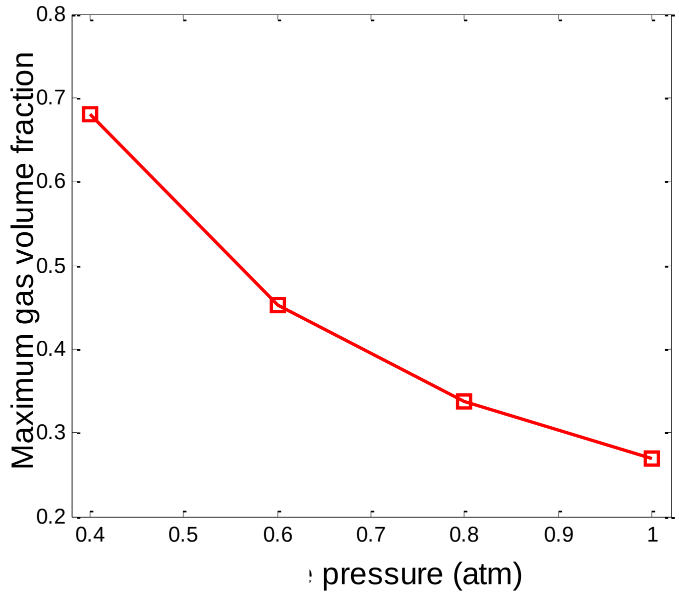




P_i=0.6atm



P_i=0.4atm



Conclusions

- In the SOM electrolysis process, the flux is highly viscous; therefore magnesium transport is significantly higher near the stirring tube during electrolysis.
  - Highest current efficiencies obtained when the stirring tube is used as cathode.

- The flow behavior of the molten flux at reduced pressure was also simulated. As the pressure of the system drops and the argon bubble size increases, the flux velocity also increases.

Acknowledgement

- The authors thank Dr. Adam C. Powell, Steve Tucker, and Dr. Soobhankar Pati for helpful discussions.

Thank you for your attention!

Questions & Comments?