



Flows and mass transfers in two superimposed liquid layers in an induction furnace



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ABSTRACT

In foundry, induction furnace is a well-known, clean, energy-efficient and well-controllable melting process. In order to improve its refining capacity, a salty or oxide liquid layer can be added at the surface of the liquid metal. This paper aims to simulate numerically mass transfers that occur at the liquid–liquid interface between these two liquid layers. To achieve this, the flows in both salty and metallic phases are calculated, taking into account all the present phenomena in the bulks (i.e. electromagnetic stirring, buoyancy, turbulence, heat transfer), as well as those at the interface (i.e. electromagnetic shaping, viscous shear driving). Comparison is made with literature experimental measurements.

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1. Introduction

The metal-refining step in metallurgy, or in spent nuclear fuels reprocessing, is based on a liquid–liquid extraction that aims to transfer a pollutant from one phase to another. In the reactor, two immiscible liquid layers (a metallic phase lying below a salty or an oxide phase) are separated by an interface where mass exchange occurs via redox reaction. Kinetics of mass transfer, as well as its overall rate, are strongly dependent on the motions in the two layers, as well as the motion of the interface itself. Thus, stirring reduces mass transfer resistances by:

- promoting the renewal of species in the vicinity of the interface by advection in the bulk of both phases,
- increasing the apparent diffusion thanks to the contribution of turbulence with, correspondingly, a decrease of the thickness of the diffusion sub-layers.

Numerical simulation is of great help to optimise such reactors. However, although mass transfers through an interface separating a liquid metal and a molten salt or oxide are at the heart of metallurgical processes, we do not find a satisfactory description of such transfers in the literature.

The computation of an entire reactor is a tough task, not only because like in mass transfers description, but also because it involves strongly coupled physical phenomena. In this article, we present a pragmatically conducted study. The choice of each model

is explained and limitations are highlighted. We applied to validate each of the selected models.

After a brief description of a pyrometallurgical reactor able to promote such mass transfers, we focus on the various physical phenomena and quantify them. Then, the strategy chosen to perform the simulation is explained. The implementation of coupling between the two fluid flows is presented, and a focus is made on the numerical description of the interfacial shear stresses. The modelling choices attached to this description are validated on a simple flow (i.e. two-layers laminar plane Couette flow), whose analytical expression is easy to derive. Stationary flows in the studied reactor are then presented and the promoted mass transfers are calculated finally as a post-process. The time-dependent concentration of the pollutant in the metallic phase is compared with experimental results from the literature.

2. Simulated reactor and attached physical phenomena

A sketch of the experimental reactor is shown in Fig. 1. It corresponds to a reactor described by Perrier [1]. Two liquid layers are lying in a graphite crucible located in an electromagnetic field generated by a 6-turn coil. The internal radius of the crucible is $a = 4.5$ cm. The thicknesses of the metallic and salty layers are 4 and 2 cm, respectively.

This configuration has been used by Saadi [2], to study mass transfer of cerium from a fluoride molten salt to a metallic alloy. The respective chemical compositions of each phase are *Sb–Li* (10 mol.%) and *LiF–CeF₃* (2 mol.%) for the metallic and salty layers. The physical properties of involved materials are summarized in Tables 1 and 2. These properties are assumed to be constant; i.e.

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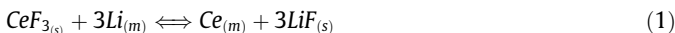
Nomenclature

a	internal radius of the graphite crucible [m]	T_s	mean temperature in the molten salt layer [K]
A	magnetic potential [T m]	T_{wk}	mean temperature of wall k [K]
B	magnetic field [T]	\mathbf{u}	velocity field [m s^{-1}]
B_0	characteristic value of the magnetic field [T]	U_A	Alfven velocity [m s^{-1}]
$C_{p,i}$	specific heat capacity of the phase i [$\text{J kg}^{-1} \text{K}^{-1}$]	$U_{s,b}$	characteristic velocity in the salty layer owing to natural convection [m s^{-1}]
$D_{j,i}$	diffusion coefficient of the species j in the phase i [$\text{m}^2 \text{s}^{-2}$]	$U_{s,s}$	characteristic velocity in the salty layer owing to viscous driving [m s^{-1}]
f	frequency of the inducing current [Hz]	U_m	characteristic velocity in the metallic layer owing to electromagnetic stirring [m s^{-1}]
f_{int}	force density imposed in the first interfacial cells [N m^{-3}]	x_j	mass fraction of the j -species
F_b	thermo-gravitational force density [N m^{-3}]	Greek symbols	
F_{em}	electromagnetic force density [N m^{-3}]	α	volume fraction function
h	heat transfer coefficient [$\text{W m}^{-2} \text{K}^{-1}$]	β_s	thermal expansion coefficient of the salt [K^{-1}]
h_{em}	dome height [m]	ε	dissipation rate of turbulent kinetic energy [$\text{m}^2 \text{s}^{-3}$]
g	gravity [m s^{-2}]	$\delta_{em, i}$	electromagnetic skin depth in the phase i [m]
I_{rms}	coil current rms value [A]	Φ_k	convective heat flux at surface k [W]
J_k	radiosity of surface k [W m^{-2}]	φ_k	radiative heat flux density at surface k [W m^{-2}]
k	turbulent kinetic energy [$\text{m}^2 \text{s}^{-2}$]	λ_i	thermal conductivity of the phase i [$\text{W m}^{-1} \text{K}^{-1}$]
k_B	Boltzmann constant [J K^{-1}]	μ_0	vacuum permittivity [H m^{-1}]
N_A	Avogadro number [mol^{-1}]	μ_i	dynamic viscosity of the phase i [Pa s]
Nu	Nusselt number	μ_t	turbulent dynamic viscosity [Pa s]
Pr	Prandtl number	ρ_i	density of the phase i [kg m^{-3}]
Ra	Rayleigh number	σ_B	Stefan–Boltzmann constant [$\text{W m}^{-2} \text{K}^{-4}$]
Re	Reynolds number	σ_i	electrical conductivity of the phase i [$\Omega^{-1} \text{m}^{-1}$]
R_m	magnetic Reynolds number	τ_{int}	interfacial shear stress [N m^{-1}]
R_ω	shield parameter	χ	Joule power density [W m^{-3}]
Sc	Schmidt number	ω	E.M. field angular frequency [rad s^{-1}]
t	time [s]		
T	temperature [K]		
T_0	ambient argon temperature [K]		

not temperature dependent (except for the argon and salt density), and are chosen at the bath temperature (950 °C). The way diffusion coefficients are evaluated is described in Appendix 1.

2.1. Liquid–liquid extraction at the interface

At the salt–metal interface, lithium ($\text{Li}_{(m)}$), initially present in the metallic layer, reduces cerium fluoride ($\text{CeF}_{3(s)}$) from the molten salt ($\text{LiF}_{(s)}$) into metallic cerium ($\text{Ce}_{(m)}$). As a consequence, cerium is transferred from the salty to the metallic layer, owing to the following oxydo-reduction reaction that occurs at the interface.



In such extraction processes, as in many other chemical reactors, the kinetic of transfer can be governed by reaction rate or by mass transfers. Indeed, the overall rate of transfer will depend on three main steps, which are:

- the transport of reactants to the reaction site; i.e. to the interface between the two fluids
- the chemical reaction at the interface
- the transport of products away from the reaction site

However, for metallurgical applications, the rate-determining step is, mostly, the mass transfer and not the kinetic of the chemical interfacial reaction. The model used to describe these transfers is explained in the next section.

2.2. Diffusion-limited kinetics model

Several models can describe the mass transport of reactants and products to and away from the interface. Here, the mass transfer coefficient is deduced from a simple theory for interfacial mass

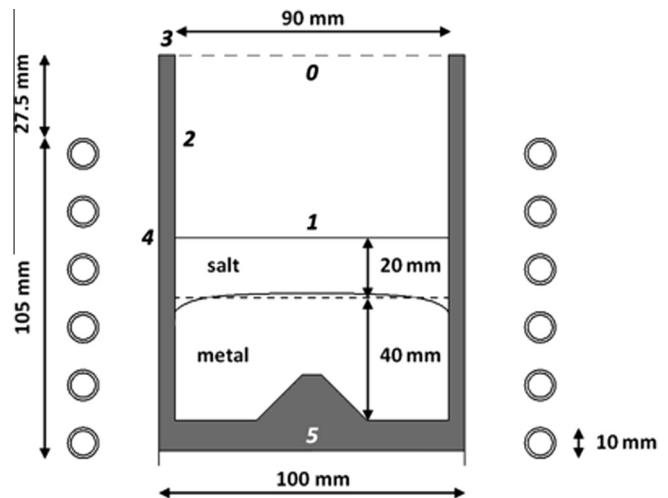


Fig. 1. Sketch of the studied configuration.

transfers, developed by Lewis and Whitman [3]: the thin-film theory. This model assumes that mass transfers are only limited by molecular diffusion near the interface, while convection dominates away from these chemical layers. Thus, two kinds of region can be defined (Fig. 2):

- a chemical diffusion layer also called ‘stagnant film’, where mass transfer occurs thanks to molecular diffusion
- a well-mixed region where the concentration is the same in the all bulk and only time-dependent

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