

# An Algebraic Approach to Modeling Distributed Multiphysics Problems: the case of a DRI Reactor<sup>\*</sup>

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**Abstract:** This paper deals with the problem of modelling a chemical reactor for the Direct Reduction of Iron ore (DRI). Such a process is being increasingly promoted as a more viable alternative to the classic Blast Furnace for the production of iron from raw minerals. Due to the inherent complexity of the process and the reactor itself, its effective monitoring and control requires advanced mathematical models containing distributed-parameter components. While classical approaches such as *Finite Element* or *Finite Differences* are still reasonable options, for accuracy and computational efficiency reasons, an *algebraic* approach is proposed. A full multi-physical, albeit one-dimensional model is addressed and its accuracy is analysed.

*Keywords:* Direct Reduction of Iron ore; Steel industry; Modelling.

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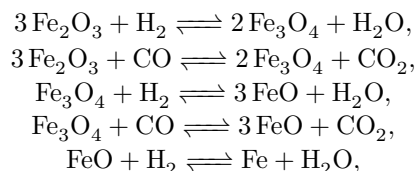
## 1. INTRODUCTION

In the recent years, the need of improving the efficiency, productivity, and safety of the steelmaking process has become more urgent, due to rising production costs and to restrictions imposed by environmental regulations. One of the increasingly successful routes for steelmaking, is the gas-based Direct Reduction of Iron Ore (DRI), which is a greener and more energy-efficient alternative to the classical Blast Furnace or Reduction Furnace/Melting Furnace processes. In fact, while the primary energy source for the classical processes is coal, in the DRI case not only coal, but Natural Gas, gases from coal gasification (Syngas) or coke oven gas can be used as well, leading to a reduction of emitted CO<sub>2</sub> that can range from 40% to 62% (Duarte et al. (2010)). The economic benefits are also worth noting, especially in areas where sources of natural gas are present. Due to the complexity of the process, which is a nonlinear, multi-physics, distributed-parameter system, a novel approach for advanced control and fault diagnosis schemes for such a system is needed. This is particularly important since a typical plant produces 200 ton/hour of DRI and the cost for steel products is around 500 Eur/ton: by considering an efficiency in the conversion of DRI to finished steel products of 85%, it means that shutdown costs may reach 2 MEur per day. In this paper, we address the foundations of those problems, by proposing a novel model for the DRI process based on the algebraic formulation. In Section 2, the DRI process is described, while in Section 3 we explain why a new model is necessary and we introduce the Algebraic Formulation approach, which we use in Section 4 to develop the DRI

model. In Section 5, some simulation results are given. Some concluding remarks are finally provided in Section 6.

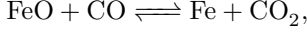
## 2. THE DRI PROCESS

The DRI (Direct Reduction Iron) process is a complex chemical process, converting lump ore and/or iron oxide pellets into highly metallised, stable iron product. The reactions are obtained by letting circulate a reducing gas, mainly constituted by hydrogen and carbon monoxide, through a moving bed of particulate iron ore at temperatures on the order of 700°C to 1000°C (Zervas et al. (1996)), following one of the two most successful DRI commercial solution: the MIDREX and the ENERGIRON (Kolbeinsen (2010)). The reactions happen inside a shaft reactor, that can reach pressure values of about 6 bar and temperature as high as 1100 degrees C. In these conditions, more typical of chemical, rather than steel plants, safety issues should be considered very carefully in the DRI plant design, to avoid injuries, environmental damage or plant damage, as well as to maximize throughput (Gonzalez Lopez and Noriega (2008)). As in Zugliano et al. (2013), a one-dimensional model will be considered here. Each cell is modeled taking into account pellet and gas flows, mass/molar concentration and thermal energy transport, heat exchange between gas and solid phases, and chemical reactions, making it a multi-physics problem. The following chemical reactions are considered: the reduction reactions

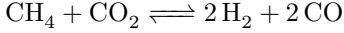
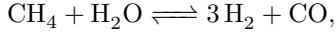


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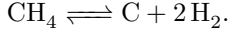
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the steam reforming



and the methan cracking



### 3. THE ALGEBRAIC FORMULATION

Due to the large dimensions of the reactor and the significant gradients expected, it is natural to model it as a distributed-parameters system (Parisi and Laborde (2004); Nouri et al. (2011); Zugliano et al. (2013)). A classical approach is to rely on some PDE discretization such as FDTD, FEM or FV. In this paper an Algebraic Formulation (AF) approach will be followed, which avoids entirely the discretization step by using algebraic equations in first place (Ferrari et al. (2013); Tonti (2001, 2013)). The AF, as well as other direct algebraic methods such as DEC (Desbrun et al. (2005)), MD (Bossavit (1998)) or FIT (Clemens and Weiland (2001)), presents many advantages, and leads to a structure-preserving and conservative numerical scheme.

The AF makes use of *global variables*, that is, variables associated not to a point, like field variables in differential theories, but to a finitely-sized domain. For instance, a global variable in electromagnetism is the magnetic flux through a surface, which is measured in  $\text{Wb}$ , whereas a field variable is the magnetic flux density at a point on the surface, measured in  $\text{Wb m}^{-2}$ . Global variables can be divided in three main categories: *configuration v.*, which define the state of a system; *source v.*, which describe all the causes that can change the configuration; and *energy v.*, which can be computed from the previous two. Variables, as usual, are linked by equations, namely: *definition eq.*, *balance eq.* and *constitutive eq.*. The key point of the AF is the association of variables to a discrete space and time reference framework, called a *complex* (Munkres (2000)). The complex (see Fig. 1) is made up of oriented finite geometric elements, the *p-cells*, with  $p \in \{0, \dots, 3\}$  being the geometric dimension, which are denoted with the letters **I** (time instants), **T** (time intervals), **P** (points), **L** (lines), **S** (surfaces), and **V** (volumes), and can be endowed with either an *internal* or an *external* orientation, in the latter case a tilde being used. For a generic variable  $a$ , the notation  $a[\mathbf{I}, \mathbf{P}]$  denotes for instance its association with the time element **I** and the spatial one **P**, while the notation  $\partial\mathbf{X}$  is used for the boundary of the generic element **X**, and  $\mathbf{X}^-$  or  $\mathbf{X}^+$  for the previous or next element when ordering is clear from the context.

In order to allow the definition of the physical variables and the equations of a given problem, the computational domain needs to be decomposed both in space and in time into two staggered complexes: the *primal* (internal orientation), and the *dual* (external orientation). An important aspect of the AF is that, even when a problem is solved in one dimension only, as in the present case, the elements of the spatial complex are anyway three dimensional entities. In our case the reactor, being an axially symmetric object, is divided into a number of stacked cylindrical frusta, the cells, along its axis (see Fig. 1).

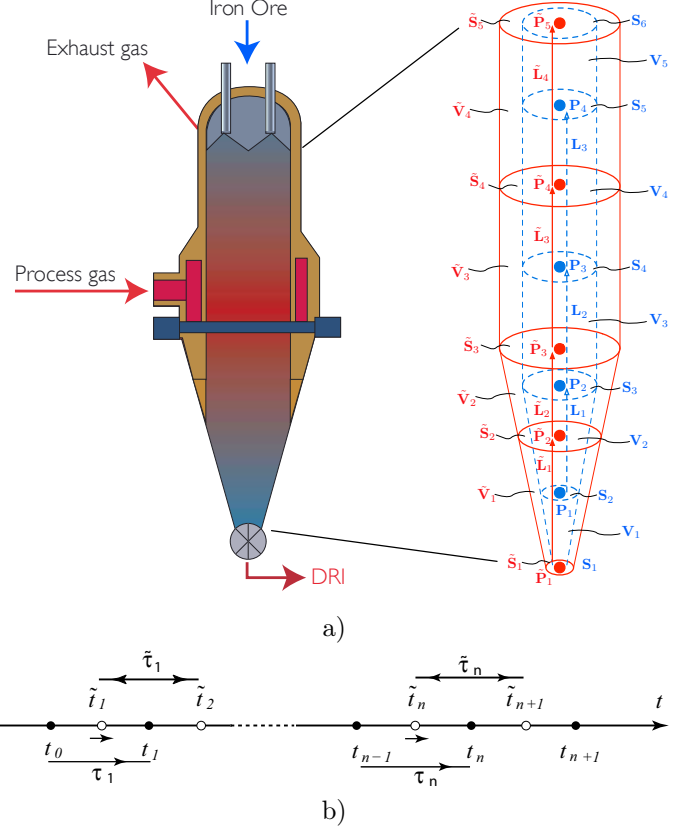


Fig. 1. a) An illustration of the of the DRI reactor, and its spatial tessellation (with only four cells for clarity), showing 0, 1, 2 and 3-cells; b) a subdivision of the time-line into primal and dual time instants  $t_i$  and  $\tilde{t}_i$ , and intervals  $\tau_i$  and  $\tilde{\tau}_i$ .

### 4. AN ALGEBRAIC MULTIPHYSICS MODEL OF A DRI REACTOR

Following the description in (Zugliano et al. (2013)), we will model three different, but fully coupled phenomena: gas and pellet flow, heat exchange, chemical reactions. We assume the following:

- plug flow, both for gas and pellet;
- quasi-static approximation for gas flow dynamics (time to reach steady state for pressures and velocities is negligible)
- instantaneous mixing of gas or of solid;
- heat conduction and concentration diffusion is negligible;
- Unreacted Shrinking Core pellet model.

#### 4.1 Gas and pellet flow

The flow model must guarantee the conservation of mass and momentum. An Eulerian formulation will be used, and following Tonti (2013) we will associate contents to dual volumes, and flows to dual surfaces. Gas mass conservation can be easily written as

$$M_{g,\text{rate}}[\mathbf{T}, \tilde{\mathbf{V}}] = -(M_{g,\text{adv}}[\mathbf{T}, \partial\tilde{\mathbf{V}}]) + M_{g,\text{source}}[\mathbf{T}, \tilde{\mathbf{V}}] \quad (1)$$

with  $M_{g,\text{rate}}[\mathbf{T}, \tilde{\mathbf{V}}] \triangleq \frac{M_g[\mathbf{I}^+, \tilde{\mathbf{V}}] - M_g[\mathbf{I}^-, \tilde{\mathbf{V}}]}{|\mathbf{T}|}$  being the rate of change of the mass content in the generic dual 3-cell,

$$M_{g,\text{adv}}[\mathbf{T}, \partial\tilde{\mathbf{V}}] \triangleq \frac{M_g[\mathbf{I}^-, \tilde{\mathbf{V}}^-]}{|\tilde{\mathbf{V}}^-|} v_g[\mathbf{T}, \tilde{\mathbf{S}}^-] |\tilde{\mathbf{S}}^-| - \frac{M_g[\mathbf{I}^-, \tilde{\mathbf{V}}]}{|\tilde{\mathbf{V}}|} v_g[\mathbf{T}, \tilde{\mathbf{S}}] |\tilde{\mathbf{S}}|$$

the flow of mass through the boundary of that cell assuming the gas is moving upwards (see Fig. 1), and  $M_{g,\text{source}}[\mathbf{T}, \tilde{\mathbf{V}}]$  the rate of production of mass inside that cell, for instance due to chemical reactions. The conservation of gas momentum content  $\mathbf{p}_g[\tilde{\mathbf{I}}, \tilde{\mathbf{V}}]$ , instead, reads

$$\mathbf{p}_g[\tilde{\mathbf{I}}^+, \tilde{\mathbf{V}}] - \mathbf{p}_g[\tilde{\mathbf{I}}^-, \tilde{\mathbf{V}}] = \left( p_g[\tilde{\mathbf{T}}, \mathbf{P}^+] |\tilde{\mathbf{S}}^+| - p_g[\tilde{\mathbf{T}}, \mathbf{P}^-] |\tilde{\mathbf{S}}^-| \right) |\tilde{\mathbf{T}}| + I_{g,V}[\tilde{\mathbf{T}}, \tilde{\mathbf{V}}] \quad (2)$$

this last equation being simply the equivalent of the second law of motion of Newton, with  $p_g[\tilde{\mathbf{T}}, \mathbf{P}]$  being the pressure of the gas at the primal point  $\mathbf{P}$  at the center of the dual volume  $\tilde{\mathbf{V}}$  and  $I_{g,V}[\tilde{\mathbf{T}}, \tilde{\mathbf{V}}]$  the impulse of volume forces acting on the gas. An important force making up this term, apart the gravity effect, is the drag experienced by the gas flowing through the packed bed of solid pellet. In order to model this, the Ergun law (Ergun (1952)) will be employed, which relates the pressure drop along a stretch of straight pipe filled with a packed bed, to the fluid velocity. As it is an experimental law, it is very easy to write it in algebraic formulation:

$$p_g[\tilde{\mathbf{T}}, \mathbf{P}^+] - p_g[\tilde{\mathbf{T}}, \mathbf{P}^-] = \frac{150\mu|\mathbf{L}|}{D_p^2} \frac{(1-\epsilon)^2}{\epsilon^3} v_g[\mathbf{T}, \tilde{\mathbf{S}}] + \frac{1.75|\mathbf{L}|\rho_g}{D_p} \frac{(1-\epsilon)}{\epsilon^3} v_g^2[\mathbf{T}, \tilde{\mathbf{S}}] \quad (3)$$

with  $\mu$  being the gas mixture dynamic viscous friction coefficient,  $|\mathbf{L}|$  the length of the primal 1-cell representing the pipe stretch,  $\epsilon$  the bed void fraction,  $\rho_g$  the gas density and  $D_p$  the pellet equivalent diameter, with the gas quantities being referred to the undisturbed flow. Finally, we must include the gas state equation as a constitutive relation linking together the gas state variables

$$p_g[\tilde{\mathbf{T}}, \mathbf{P}] = \frac{\rho_g[\mathbf{I}, \tilde{\mathbf{V}}]}{\bar{M}_{N_g}[\mathbf{I}, \tilde{\mathbf{V}}]} RT_g[\tilde{\mathbf{T}}, \mathbf{P}] \quad (4)$$

with  $R$  being the ideal gas constant,  $\bar{M}_{N_g}[\mathbf{I}, \tilde{\mathbf{V}}] \triangleq \frac{\sum_{s \in \mathcal{S}_g} N_g^{(s)}[\mathbf{I}, \tilde{\mathbf{V}}] M_{N_g}^{(s)}}{N_g[\mathbf{I}, \tilde{\mathbf{V}}]}$  the weighted average of the molar mass, and  $N_g[\mathbf{I}, \tilde{\mathbf{V}}] \triangleq \sum_{s \in \mathcal{S}_g} N_{g,s}[\mathbf{I}, \tilde{\mathbf{V}}]$  the total number of gas moles inside the dual cell volume. The equations for the solid phase are analogous and will not be repeated, modulus the fact that this flow is assumed to be incompressible and that we neglect the drag exerted by the gas.

## 4.2 Thermal model

The thermal model allows to enforce conservation of internal energies  $U_g[\mathbf{I}, \tilde{\mathbf{V}}]$  and  $U_p[\mathbf{I}, \tilde{\mathbf{V}}]$ , by balancing all the different heat terms (see Table 2). The balance equations, remembering again that the gas and pellet flows directions are assumed to be fixed, are thus

$$U_g[\mathbf{I}^+, \tilde{\mathbf{V}}] = U_g[\mathbf{I}^-, \tilde{\mathbf{V}}] + \left( Q_{g,\text{adv}}[\mathbf{T}, \partial\tilde{\mathbf{V}}] - Q_{g,\text{conv}}[\mathbf{T}, \tilde{\mathbf{V}}] - Q_{g,\text{rad}}[\mathbf{T}, \tilde{\mathbf{V}}] - Q_{g,\text{wall}}[\mathbf{T}, \tilde{\mathbf{V}}] + \sum_{r \in \mathcal{R}} Q_{g,\text{react}}^{(r)}[\mathbf{T}, \tilde{\mathbf{V}}] \right) |\mathbf{T}| \quad (5)$$

$$U_p[\mathbf{I}^+, \tilde{\mathbf{V}}] = U_p[\mathbf{I}^-, \tilde{\mathbf{V}}] + \left( Q_{p,\text{adv}}[\mathbf{T}, \partial\tilde{\mathbf{V}}] + Q_{g,\text{conv}}[\mathbf{T}, \tilde{\mathbf{V}}] + Q_{g,\text{rad}}[\mathbf{T}, \tilde{\mathbf{V}}] + \sum_{r \in \mathcal{R}} Q_{p,\text{react}}^{(r)}[\mathbf{T}, \tilde{\mathbf{V}}] \right) |\mathbf{T}| \quad (6)$$

with  $Q_{g,\text{adv}}[\mathbf{T}, \partial\tilde{\mathbf{V}}]$  and  $Q_{p,\text{adv}}[\mathbf{T}, \partial\tilde{\mathbf{V}}]$  being computed similarly to the mass advection terms of subsection 4.1. The computation of  $Q_{g,\text{react}}^{(r)}[\mathbf{T}, \tilde{\mathbf{V}}]$  and  $Q_{p,\text{react}}^{(r)}[\mathbf{T}, \tilde{\mathbf{V}}]$  is detailed in subsection 4.3, while the other terms are computed as

$$Q_{g,\text{conv}}[\mathbf{T}, \tilde{\mathbf{V}}] = h_c A_c \left( T_g[\tilde{\mathbf{T}}, \mathbf{P}] - T_p[\tilde{\mathbf{T}}, \mathbf{P}] \right),$$

$$Q_{g,\text{rad}}[\mathbf{T}, \tilde{\mathbf{V}}] = A_c \sigma \frac{\epsilon_p}{1 - (1 - \epsilon_p)(1 - \alpha_g)} \left( \epsilon_p T_g^4[\tilde{\mathbf{T}}, \mathbf{P}] - \alpha_g T_p^4[\tilde{\mathbf{T}}, \mathbf{P}] \right)$$

$$Q_{g,\text{wall}}[\mathbf{T}, \tilde{\mathbf{V}}] = 2\pi k_w \frac{T_{wIN}[\tilde{\mathbf{T}}, \mathbf{P}] - T_{wOUT}[\tilde{\mathbf{T}}, \mathbf{P}]}{\log \frac{r_{wOUT}}{r_{wIN}}} |\tilde{\mathbf{L}}|$$

where  $h_c$  is the convection coefficient,  $A_c$  is the exchange surface,  $\epsilon_p$  and  $\epsilon_g$  are pellet and gas emissivity, respectively,  $\alpha_g$  is gas absorbance,  $k_w$  is the wall thermal conductivity,  $r_{wIN}$ ,  $r_{wOUT}$  and  $T_{wIN}$ ,  $T_{wOUT}$  are the reactor radii and the temperature, inside and outside the wall respectively,  $|\tilde{\mathbf{L}}|$  is the length of the dual 1-cell. Finally, the links between internal energies and temperatures are the constitutive equations  $U_g[\mathbf{I}, \tilde{\mathbf{V}}] = f_{U_g}(T_g[\tilde{\mathbf{T}}, \mathbf{P}])$  and  $U_p[\mathbf{I}, \tilde{\mathbf{V}}] = f_{U_p}(T_p[\tilde{\mathbf{T}}, \mathbf{P}])$  where the functions  $f_{U_g}$  and  $f_{U_p}$  represent the fact that the gas and solid heat capacities  $C_{p,g}$  and  $C_{p,p}$  are temperature dependent.

## 4.3 Chemical species balance

The chemical part of the model must enforce the conservation of the molar content for each specie:

$$N_g^{(s)}[\mathbf{I}^+, \tilde{\mathbf{V}}] = N_g^{(s)}[\mathbf{I}^-, \tilde{\mathbf{V}}] + \left( N_{g,\text{adv}}^{(s)}[\mathbf{T}, \partial\tilde{\mathbf{V}}] + \sum_{r \in \mathcal{R}} N_{g,\text{react}}^{(s)}[\mathbf{T}, \tilde{\mathbf{V}}] \right) |\mathbf{T}|, \quad \forall s \in \mathcal{S}_g \quad (7)$$

for the gas, and similarly for the solid. It is convenient here to introduce the quantity  $O_{\text{react}}^{(r)} = (K_r p_g^{(i_r)} - K'_r p_g^{(i'_r)}) A_{j_r} n_p$  that represents the number of oxygen moles reduced in an unitary volume and time by the  $r$ -th reaction, with  $K_r$  and  $K'_r$  being the direct and the inverse kinetic constants,  $i_r \in \mathcal{S}_g$  the reducing gas specie,  $i'_r \in \mathcal{S}_g$  the oxydized gas specie,  $A_{j_r}$  the contact area per pellet of the reduced solid specie  $j_r \in \mathcal{S}_p$  in the USC model, and  $n_p$  the number of pellets in an unitary volume. By

using this quantity, and the reaction equations introduced in Section 2, it is straightforward to compute the contributions of a given reaction to the terms  $N_{g,\text{react}}^{(s)}[\mathbf{T}, \tilde{\mathbf{V}}]$ ,  $N_{p,\text{react}}^{(s)}[\mathbf{T}, \tilde{\mathbf{V}}]$  and  $Q_{p,\text{react}}^{(r)}[\mathbf{T}, \tilde{\mathbf{V}}]$ . For instance, the total contribution to  $N_{p,\text{react}}^{(\text{Fe}_2\text{O}_3)}[\mathbf{T}, \tilde{\mathbf{V}}]$  is equal to  $-3(\text{O}_{\text{react}}^{(1)} + \text{O}_{\text{react}}^{(2)})|\tilde{\mathbf{V}}|$ , while the contribution to the generic term is  $Q_{p,\text{react}}^{(r)}[\mathbf{T}, \tilde{\mathbf{V}}] = \text{O}_{\text{react}}^{(r)} H_r |\tilde{\mathbf{V}}|$ , with  $H_r$  the  $r$ -th reaction enthalpy.

Table 1. Gas and pellet flow variables

Symbol <sup>1</sup>	Kind <sup>2</sup>	Description
$M_x[\mathbf{I}, \tilde{\mathbf{V}}]$	C	Mass content inside dual 3-cells
$p_g[\tilde{\mathbf{T}}, \mathbf{P}]$	C	Pressure of gas at primal 1-cells
$\rho_g[\mathbf{I}, \tilde{\mathbf{V}}]$	C	Gas density inside 3-cells
$v_x[\mathbf{T}, \tilde{\mathbf{S}}]$	S	Velocity through dual 2-cells
$M_{x,\text{adv}}[\mathbf{T}, \tilde{\mathbf{S}}]$	S	Mass flow through dual 2-cells due to advection
$M_{x,\text{react}}[\mathbf{T}, \tilde{\mathbf{V}}]$	S	Mass production rate due to chemical reactions, inside 3-cells

Table 2. Thermal model.

Symbol <sup>1</sup>	Kind <sup>2</sup>	Description
$T_x[\tilde{\mathbf{T}}, \mathbf{P}]$	C	Temperature at primal 0-cells
$U_x[\mathbf{I}, \tilde{\mathbf{V}}]$	E	Thermal energy content inside dual 3-cells
$Q_{x,\text{adv}}[\mathbf{T}, \tilde{\mathbf{S}}]$	S	Heat flux through dual 2-cells due to advection
$Q_{x,\text{react}}^{(r)}[\mathbf{T}, \tilde{\mathbf{V}}]$	S	Heat production due to chemical reaction $r \in \mathcal{R}$ , inside 3-cells
$Q_{g,\text{conv}}[\mathbf{T}, \tilde{\mathbf{V}}]$	S	Heat transfer in gas due to convection with pellet, inside 3-cells
$Q_{g,\text{wall}}[\mathbf{T}, \tilde{\mathbf{V}}]$	S	Heat transfer in gas due to convection with reactor walls, inside 3-cells
$Q_{g,\text{rad}}[\mathbf{T}, \tilde{\mathbf{V}}]$	S	Heat transfer in gas due to thermal radiation, inside 3-cells

#### 4.4 Resolution scheme

A clear advantage of the AF is that it leads in a natural way to explicit time marching schemes (Ferrari et al. (2013); Tonti (2013)), as can be verified by looking at Eqs. (1), (2), (5), (6) (7). Anyway, due to the problem being multiphysic and fully coupled, and to the presence of numerous parameters that are temperature, pressure and concentration dependent, a scheme for solving the previous equations in the right order is needed. Furthermore, boundary conditions and initial values must be defined. In order to ease the following presentation, we will consider a one dimensional cell complex containing  $T$  primal 0-cells in time and  $N$  primal 0-cells in space, and a simplified notation will be introduced, such as

$$X(n, k) \equiv X[\cdot, \cdot]$$

where  $X$  stand for a generic variable, and  $n \in \{0, 1/2, 1, 1 + 1/2, \dots, T - 1\}$  and  $k \in \{1/2, 1, 1 + 1/2, \dots, N - 1/2\}$  are two integers which identify in time and space the cell which

<sup>1</sup> The index  $x$  can refer to either gas ( $g$ ) or solid ( $p$ )

<sup>2</sup> C = configuration, S = source, P = parameter, E = energy

the variable is referred to. In particular, integer values of  $n$  are used for referring to primal instants or their corresponding dual interval, while fractional values for primal intervals or their corresponding dual instants. Similarly, integer values of  $k$  are used for primal points, dual lines, primal surfaces or dual volumes, and fractional values for dual points, primal lines, dual surfaces or primal volumes. The chosen boundary conditions will constrain the value of the gas velocity, pressure, temperature and composition at the gas inlet, and the solid velocity, temperature and composition at the upper inlet, as in practice these values are known and/or measurable on line. As initial conditions, a uniform temperature, pressure and nominal composition, representing a cold reactor, will be chosen. Considering the modelling assumptions, at the generic  $n$ -th time instant the resolution scheme will comprise the following steps, in order to compute the new state of the gas phase (the procedure is analogous for the solid phase)

- (1) The pressures  $p_g(n, k)$  are computed from eq. (2), and from (3) and  $v_g(n - 1/2, k - 1/2)$ , starting from the bottom boundary value  $p_g(n, 1)$  and moving upwards in the reactor;
- (2) The mass content  $M_g(n, k)$ , the internal energy  $U_g(n, k)$  and the molar content  $N_g(n, k)$  are updated using eqs. (1), (2) and (7), and the source terms referred to the time interval  $n - 1/2$
- (3) The temperature  $T_g(n, k)$  is computed as  $T_g(n, k) = T_g(n - 1, k) + \frac{U_g(n, k) - U_g(n - 1, k)}{C_{g,p}(n - 1/2, k)}$  by applying the definition of heat capacity  $C_{g,p}$ ;
- (4) All the physical parameters that are time varying are updated (such as gas density, heat capacity, viscosity, absorbance, etc ...)
- (5) The gas velocity  $v_g(n + 1/2, k + 1/2)$  is computed from  $v_g(n + 1/2, k - 1/2)$  and eq. (1) and (4), starting from the bottom boundary value  $v_g(n + 1/2, 1/2)$  and moving upwards in the reactor;
- (6) All the advection terms referred to the time interval  $n + 1/2$  are computed

Table 3. Chemical species balance.

Symbol <sup>1</sup>	Kind <sup>2</sup>	Description
$N_g^{(s)}[\mathbf{I}, \tilde{\mathbf{V}}]$	C	Molar content of gas specie $s \in \mathcal{S}_g \triangleq \{\text{H}_2, \text{CO}, \text{H}_2\text{O}, \text{CO}_2, \text{CH}_4, \text{N}_2\}$ inside dual 3-cells
$N_p^{(s)}[\mathbf{I}, \tilde{\mathbf{V}}]$	C	Molar content of solid specie $s \in \mathcal{S}_p \triangleq \{\text{Fe}_2\text{O}_3, \text{FeO}, \text{Fe}, \text{C}, \text{Gangue}\}$ inside dual 3-cells
$T_x[\tilde{\mathbf{T}}, \mathbf{P}]$	C	Temperature at a primal 0-cells
$p_g[\tilde{\mathbf{T}}, \mathbf{P}]$	C	Pressure of gas mixture at primal 1-cells
$p_g^{(s)}[\tilde{\mathbf{T}}, \mathbf{P}]$	C	Partial pressure of gas specie $s \in \mathcal{S}_g$ at primal 1-cells
$M_{N_x}^{(s)}$	P	Molar mass of specie $s$
$N_{x,\text{react}}^{(s)}[\mathbf{T}, \tilde{\mathbf{V}}]$	S	Molar production rate of specie $s$ due to chemical reactions, inside 3-cells
$Q_{x,\text{react}}^{(r)}[\mathbf{T}, \tilde{\mathbf{V}}]$	S	Heat production due to chemical reaction $r \in \mathcal{R}$ , inside 3-cells

- (7) All the source terms due to chemical reactions, or heat transfer, are computed.

As it can be seen, steps from 1) to 4) are needed for updating configuration and parameter variables to the actual time instant, using the source terms of the previous interval; steps 5) to 7) are needed, instead, for computing the source terms for the next time interval. A problem that can arise in “closing” all the equations with this scheme, is that due to the nonlinearity of the constitutive eq. (4) and/or of the time varying parameters, the gas density predicted by eq. (1) may not be consistent with eq. (4), especially during transients. In order to maintain this discrepancy at a negligible level, a prediction/correction approach is introduced in step 5), so that the computed velocity is corrected in order to account for the gas expansion or contraction predicted by eq. (4). Similar approaches are common in numerical modelling of compressible fluid flow (see for instance Xiao (2004); van der Heul et al. (2003)) and in the present case the proposed correction has proved to make the gas densities converge in a small number of iterations, as will be shown in the next section.

## 5. SIMULATION RESULTS

In this section, we illustrate the effectiveness of the proposed approach by analyzing the simulation behaviour of a "toy model" with only 4 cells. In figure 2, we analyze the dynamics of the molar fractions, both for gas and pellet, along the four cells during the length of the simulation. After that, we checked moles balances (see an example in Fig. 3), by computing:

$$N_{in}(n, k) = \sum_{m=0}^{n-1} N_{flow}(m + 1/2, k - 1/2)$$

$$N_{out}(n, k) = - \sum_{m=0}^{n-1} N_{flow}(m + 1/2, k + 1/2)$$

$$N_{react}(n, k) = \sum_{m=0}^{n-1} N_{chem}(m + 1/2, k)$$

$$N_{store}(n, k) = N(n, k)$$

Finally, we verified energy balance checks (see Fig. 4).

## 6. CONCLUDING REMARKS

In this paper, we developed a new model for the DRI process based on the Algebraic Formulation. This work will pave the base for advanced Model-Based Control or Model-Based Fault Diagnosis schemes. As a future work we are going to simulate and validate a 160 cells model and we are going to study some faulty scenarios. The objective is the implementation of a distributed monitoring architecture Ferrari et al. (2012); Boem et al. (2013), by considering each cell as a subsystem. One of the main challenges, apart from the complexity of the chemical plant, is that there are only few sensors in the real process, measuring only some of the state variables (input and output of the reactor) and so the behavior of gas and pellet in the internal cells has to be reconstructed.

## REFERENCES

- Boem, F., Ferrari, R.M., Parisini, T., and Polycarpou, M.M. (2013). Distributed fault diagnosis for continuous-time nonlinear systems: The input–output case. *Annual Reviews in Control*, 37(1), 163–169.
- Bossavit, A. (1998). *Computational electromagnetism*. Academic Press.
- Clemens, M. and Weiland, T. (2001). Discrete Electromagnetism with the Finite Integration Technique. *Progress In Electromagnetics Research*, 32(32), 65–87.
- Desbrun, M., Hirani, A.N., Leok, M., and Marsden, J.E. (2005). Discrete Exterior Calculus. *Arxiv preprint math/0508341*.
- Duarte, P.E., Tavano, A., and Zendejas, E. (2010). Achieving carbon-free emissions via the ENERGIRON DR process. In *AISTech*, volume 1, 165–173.
- Ergun, S. (1952). Fluid flow through packed columns. *Chemical engineering progress*, 48.
- Ferrari, R.M.G., Parisini, T., and Polycarpou, M.M. (2012). Distributed Fault Detection and Isolation of Large-scale Discrete-time Nonlinear Systems: an Adaptive Approximation Approach. *IEEE Trans. on Automatic Control*, 57(2), 275–290.
- Ferrari, R.M., Parisini, T., and Polycarpou, M.M. (2013). An algebraic approach for robust fault detection of input-output elastodynamic distributed parameter systems. In *Europ. Control Conf.*, 2445–2452.
- Gonzalez Lopez, G. and Noriega, E. (2008). Hot iron: Iron reduction technology keeps plant shutdown safe, trip free. *InTech*, 55(12).
- Kolbeinsen, L. (2010). Modelling of DRI processes with two simultaneously active reducing gases. *Steel Research Int.*, 81(10), 819–828.
- Munkres, J.R. (2000). *Topology*. Prentice Hall.
- Nouri, S., Ebrahim, H.A., and Jamshidi, E. (2011). Simulation of direct reduction reactor by the grain model. *Chemical Engineering Journal*, 166(2), 704–709.
- Parisi, D.R. and Laborde, M.A. (2004). Modeling of counter current moving bed gas-solid reactor used in direct reduction of iron ore. *Chemical Engineering Journal*, 104(1), 35–43.
- Tonti, E. (2001). A direct discrete formulation of field laws - The cell method. *Computer Modeling in Eng. and Sciences*, 2(2), 237–258.
- Tonti, E. (2013). *The Mathematical Structure of Physical Theories - A General Classification Diagram*. Springer.
- van der Heul, D.R., Vuik, C., and Wesseling, P. (2003). A conservative pressure-correction method for flow at all speeds. *Computers & Fluids*, 32(8), 1113–1132.
- Xiao, F. (2004). Unified formulation for compressible and incompressible flows by using multi-integrated moments i: one-dimensional inviscid compressible flow. *Journal of Computational Physics*, 195(2), 629–654.
- Zervas, T., McMullan, J., and Williams, B. (1996). Gas-based direct reduction processes for iron and steel production. *Int. Journal of Energy Research*, 20(2), 157–185.
- Zugliano, A., Primavera, A., Pignattoni, D., and Martinis, A. (2013). Online modelling of energiron direct reduction shaft furnaces. In *IFAC Int. Symp. on Control, Opt. and Automation in Mining, Minerals and Metal Proc.*

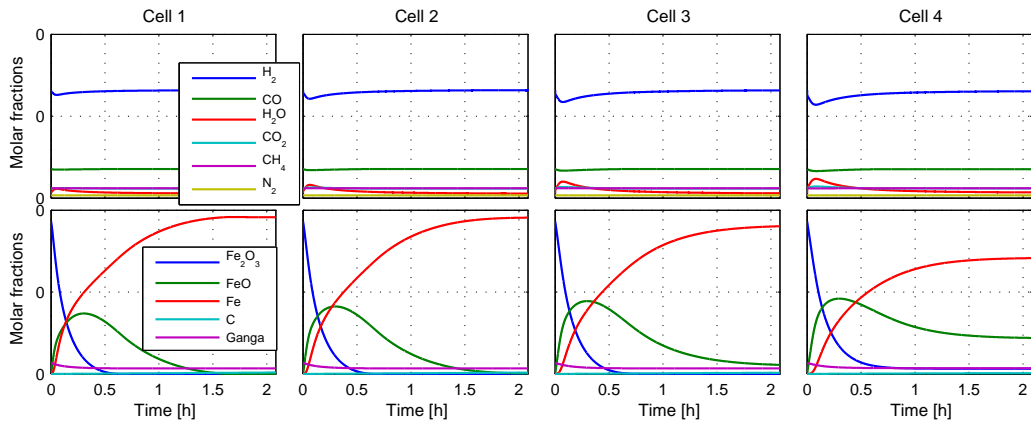


Fig. 2. Molar fractions dynamics for gas and pellet species in the four cells.

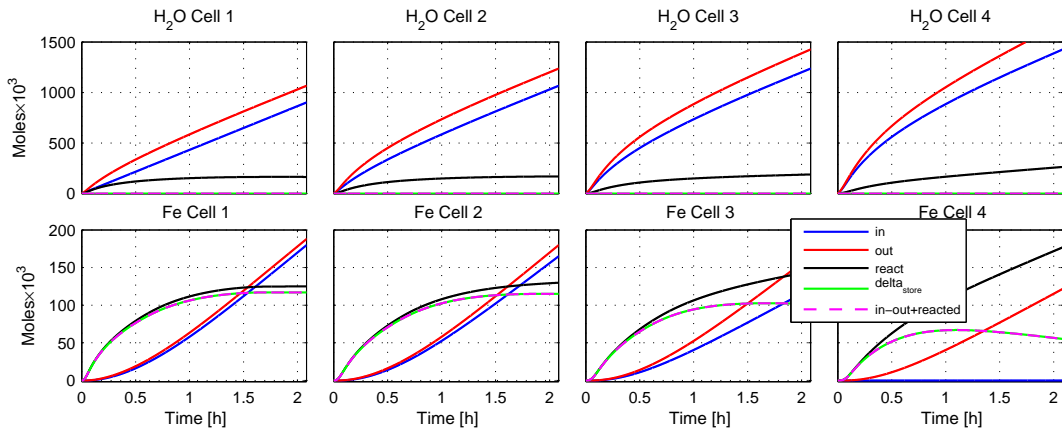


Fig. 3. Mole balance checks for two elements (steam and iron) in the four cells.

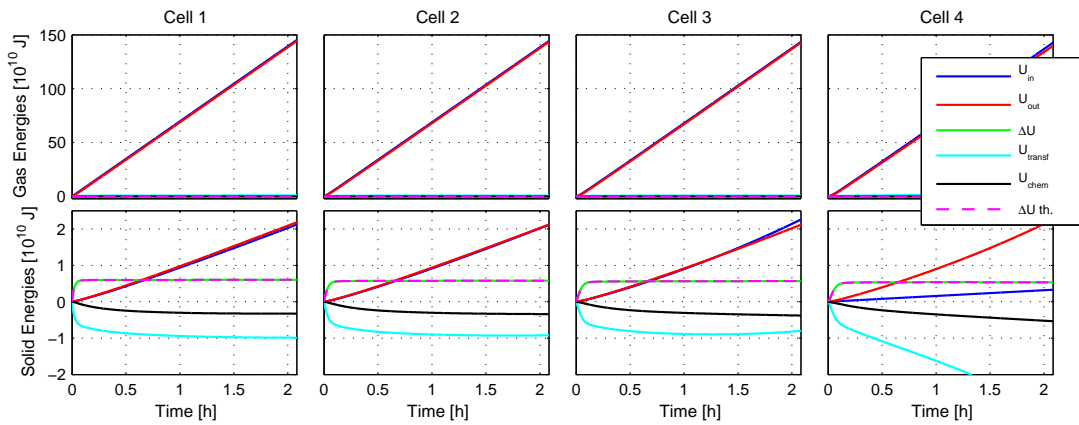


Fig. 4. Energy balance checks for gas and pellet species in the four cells.