

**ENERGY BASED DISCRETIZATION OF AN  
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Abstract: A new method for the spatial discretization of complex multi-scale systems described by partial differential equations is presented. This method allows to preserve the global power balance equation and the geometric structure of the system. The modelling of the adsorption column is based on a network approach. The key notions are the energy function and the description of the power transfers within the system and through its boundaries with the help of a power-conserving geometric structure. The proposed discretization method preserves this geometric structure and is thermodynamically consistent.

Keywords: Energy based Modelling, Distributed parameter systems, Discretization

**1. INTRODUCTION**

An adsorption column is a complex system which may be mathematically described by multi-scale partial differential balance equations. It may also be modelled using a network approach. This approach, which is an extension of the infinite dimensional port based modelling approach, consists in splitting each phenomena into atomic elements with particular energetic behaviors. Then, these atomic elements are connected via an *interconnection* structure which characterizes energy exchanges within the system and through its boundaries. This kind of modelling presents many advantages compared to the classical PDEs approach. First of all, each *atomic* element is well characterized from an energetic point of view. The interconnection between these *atomic* elements is done using power conjugated variables, named the port variables. The use of these port variables makes the interconnection between elements from

different physical domains consistent. As a consequence, the second advantage of such modelling is the modularity that it offers. Submodels and laws can be changed without taking into account problems linked to the interconnection : causality, consistency of the port variables etc ... Finally the third advantage that particularly interests us and that is the center of interest of this paper is the discretization method that derives directly from this formalism. This spatial discretization method preserves the energetic behavior of each subsystems, the geometry of the energy flows and the global power balance.

The main phenomena that occurs within the column (diffusion, mixing and convection) can be represented using a conservative part, a dissipative part and an interconnection structure named "Dirac structure" which is also used in the Port Hamiltonian Systems definition (Golo *et al.*, 2004; Maschke and Schaft, 2001; Schaft

and Maschke, 2002). This representation is related respectively to energy conservation, passivity and instantaneous power conservation. These underlying properties are fundamental in control theory since they may be used for stability analysis or control purposes.

Finite dimensional approximation is a fundamental concern for the control of distributed parameters complex systems. One of the difficulties is to develop a reduction method which preserves some interesting qualitative features of the original model (such as stability, passivity, etc.). In this paper, we present a method of spatial discretization for an adsorption column model. One of the interests of this method is that the Dirac structure is preserved as well as the associated global power balance equation.

In section 2, we briefly recall some basic features of port-based modelling. In section 3 we introduce the adsorption model and give its associated multi-scale geometric model. The section 4 is devoted to the presentation of the discretization method. The section 5 presents some simulation results issued from this discretization scheme.

## 2. PORT BASED MODELLING FOR DISTRIBUTED SYSTEMS

In this section we recall the main differences between the classical and the port based modelling approaches. The port based modelling is using a network type language. This kind of approach takes place within an unified approach for the energetic modelling of complex multidomain systems. Let us restrict the presentation to matter conservation. In this case, the general mass balance equations for species  $i$  in a 3-dimensional spatial domain  $V$  issued from the conservation laws take the familiar form:

$$\int_V \frac{\partial q_i}{\partial t} = - \int_V \operatorname{div}(N_i) \ , \forall i \in \{1, \dots, n_c\} \quad (1)$$

where  $n_c$  denotes the number of components,  $q_i$  the molar density or concentration,  $N_i$  the molar flux of the specie  $i$  going through the boundary  $\partial V$  of the domain  $V$ . A distributed source term  $f_i$  may appear in the balance equation but is omitted here as it is not useful to outline the instantaneous power preserving interconnection structure. Let denote  $d$  the exterior derivative of a differential form and note that the previous mass balance equation can be written in the local form :

$$\frac{\partial q_i}{\partial t} = -dN_i \ , \forall i \in \{1, \dots, n_c\} \quad (2)$$

The port based modelling defines the network variables according to the Gibbs equation. Let  $g$

denotes the Gibbs free energy density. We assume that this specific energy depends on the molar concentration vector, *i.e.*  $g = g(q)$ . The time variation of the total Gibbs free energy can be written ( $\delta_c g$  denotes the variational derivative of  $g$ ) :

$$\frac{\partial}{\partial t} \int_V g = \int_V (\delta_c g)^T \wedge \dot{q} \quad (3)$$

Using the mass balance equation (2) the global Gibbs equation becomes :

$$\frac{\partial}{\partial t} \int_V g = - \int_V (\delta_c g)^T \wedge dN \quad (4)$$

and after integration by parts of the right hand term :

$$\int_V (\delta_c g)^T \wedge dN + \int_V d((\delta_c g)^T) \wedge N = \int_{\partial V} (\delta_c g)^T \wedge N \quad (5)$$

The network variables are then defined as the pairs  $(\delta_c g, dN)$  and  $(d(\delta_c g), N)$ . The variables  $\delta_c g = \mu_i = e_1$  and  $d(\delta_c g) = d\mu = e_2$  are called the *effort variables* and the variables  $dN = \Phi_1$  and  $N = \Phi_2$  are called the *flow variables*. The pair of effort and flow variables is called power conjugated variables as their product has the unit of a power. Consequently, the equation (5) links the power within the spatial domain and the power flux at the boundary. With these notations the interconnection structure can be written

$$\begin{pmatrix} \Phi_1 \\ e_2 \end{pmatrix} = \begin{pmatrix} d & 0 \\ 0 & d \end{pmatrix} \begin{pmatrix} \Phi_2 \\ e_1 \end{pmatrix} \quad (6)$$

In addition to the equation (6) we define the boundary variables by :

$$\Phi_\partial = -\Phi_2|_{\partial V} \quad , \quad e_\partial = e_1|_{\partial V} \quad (7)$$

Using these notations, we can state that  $((e_1, e_2), (\Phi_1, \Phi_2), e_\partial, \Phi_\partial)$  defines a *Dirac structure* (See (Schaft and Maschke, 2002), (Maschke and Schaft, 2001) for details).

## 3. THE PORT BASED MODEL OF AN ADSORPTION COLUMN

Adsorption processes are multi-scale processes. If a zeolite is used as adsorbent medium, the mass transfer phenomena description may be decomposed at three different scales namely the extra-granular, macroporous and microporous scales (see Fig. 1).

In this section we present the port-based model of the microporous scale and the coupling with the macroporous scale. The two other scales models are similar and not detailed in this paper. Furthermore all the considered models are isothermal and we assume that only one of the components is diffusing at the microporous scale.

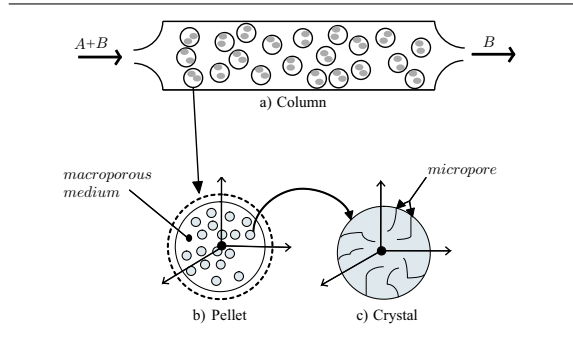


Fig. 1. Adsorption column

In the context of a three-dimensional spatial domain, we distinguish between zero-forms (functions), one-forms, two-forms and three-forms. Basically functions such as  $\mu_i$  can be evaluated at any point of the spatial domain, one-forms can be integrated over every 1-dimensional curve, two-forms such as molar flux  $N_i$  (of species  $i$ ) can be integrated over every 2-dimensional surface and three-forms such as concentrations  $q_i$  can be integrated on every sub-volume of the spatial domain.

In the following we consider a spherical symmetry in spherical coordinates  $(r, \theta, \phi)$ . Consequently :

- the molar flux may be reduced to the 0-form (on a 1D domain)  $\phi_{i2}^{mic}$  such that  $\phi_{i2}^{mic} = 4\pi r^2 N_i^{mic}$ ,
- the chemical potential of species  $i$ , the 0-form  $\mu_i^{mic}$  becomes the 0-form denoted by  $e_{i1}^{mic}$ ,
- the concentration of species  $i$ , the 3-form  $q_i$  becomes the 1-form denoted by  $q_i^L = 4\pi r^2 q_i$ .

Let now consider the figure Fig. 2 and first the left hand part of the picture relative to the conservation phenomenon.

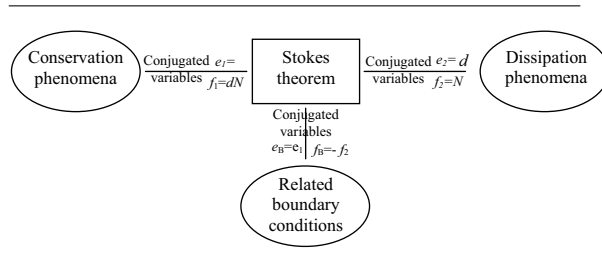


Fig. 2. Energy based model of the microporous scale

The conserved variable is the linear concentration of species  $i$ , the 1-form  $q_i^L$ , which obeys the conservation equation:

$$\frac{\partial q_i^L}{\partial t} = -\text{div} \phi_{i2}^{mic} = -\phi_{i1}^{mic} \quad (8)$$

The closure equation representing the thermodynamical equilibrium in the adsorbed scale is derived from a Langmuir's model such as ( $*$  denotes the Hodge star product which, in the one-

dimensional case, transforms 0-forms into 1-forms and conversely) :

$$e_{i1}^{mic} = \mu_i^0(T, P_0) + RT \ln \left( \frac{1}{P_0 k} \frac{*q_i^L}{*q_i^L - *q_i^L} \right) \quad (9)$$

Let now consider the right hand part of the picture of Fig. 2 that represents the diffusive phenomenon. Maxwell-Stefan law is used for representing the diffusion in the microporous scale. The only considered friction is the one exerted by the solid on species  $i$ . In this case, the Maxwell-Stefan law becomes:

$$\phi_{i2}^{mic} = -\frac{D^{mic} *q_i^L}{RT} \frac{\partial e_{i1}^{mic}}{\partial r} = -\frac{D^{mic} *q_i^L}{RT} *e_{i2}^{mic} \quad (10)$$

Equations (10) and (8) make appear the interconnection structure depicted in the center of the figure Fig. 2 and defined by :

$$\begin{cases} \phi_{i1}^{mic} = \frac{\partial \phi_{i2}^{mic}}{\partial r} \\ e_{i2}^{mic} = \frac{\partial e_{i1}^{mic}}{\partial r} \end{cases} \quad (11)$$

We also define some *port variables* as :

$$\phi_B = -\phi_{i2| \partial}, \quad e_B = e_{i1| \partial} \quad (12)$$

The flow variables  $(\phi_{i1}^{mic}, \phi_{i2}^{mic})$  and the effort variables  $(e_{i1}^{mic}, e_{i2}^{mic})$  are respectively the extensive and intensive variables.  $(\phi_{i1}^{mic}, e_{i1}^{mic})$  and  $(\phi_{i2}^{mic}, e_{i2}^{mic})$  are two couple of power conjugated variables. This interconnection structure is power preserving and makes the link between the energy within the spatial domain and the boundary power flows. In the case of crystal, the power flux at the boundaries is composed with power flux in the center of the crystal and power exchanges with the macroporous medium.

The coupling between microporous and macroporous scales is done using two kinds of variables, the intensive and extensive variables. The coupling relation between the intensive variables is derived from the assumption of local equilibrium at the interphase between the two scales. This leads to:

$$\mu_i^{mic}(x, z)|_{z \in \partial V^{mic}} = \mu_i^{mac}(x) 1_{\partial V^{mic}(x)}(z) \quad (13)$$

where  $1_{\partial V^{mic}(x)}(z)$  denotes the function taking the value 1 if  $z \in \partial V^{mic}(x)$ , 0 else. Another coupling relation is defined on the conjugated extensive variables, the volumetric density flux variable at the macroporous scale  $f_i^{mac}(x)$  and the flux variable of microporous scale  $N_i^{mic}(x, z)|_{z \in \partial V^{mic}}$  restricted to the boundary of its domain. This coupling relation between the extensive variables

is the volumetric mass balance equation which expresses the continuity of molar flux at the boundary of the two scales at the point  $x \in V^{mac}$  :

$$f_i^{mac}(x) + \left( \int_{\partial V^{mic}(x)} N_i^{mic}(x, z) dS(z) \right) \cdot \rho_p(x) = 0 \quad (14)$$

with  $\rho_p(x)$  the *volumetric density* of crystals in the pellet.

#### 4. DISCRETIZATION

We shall follow the discretization procedure based on a mixed finite element method and adapted to Port Hamiltonian systems in (Golo *et al.*, 2004). The purpose is to preserve the energetic behavior of each basic element of the figure Fig. 2. For that purpose, we propose appropriated interpolation functions for both effort and flow variables.

##### 4.1 Approximation of flows and efforts

In the sequel we shall derive a discretized power conserving structure for a finite element defined on some radial interval  $\mathcal{R} = [a, b] \subset Z = [0, R_{mic}]$ . Hence the port variables of such a finite element are:

$$\begin{aligned} e_{\partial}^a(t) &= e_1(t, a) & e_{\partial}^b(t) &= e_1(t, b) \\ \phi_{\partial}^a(t) &= -\phi_2(t, a) & \phi_{\partial}^b(t) &= -\phi_2(t, b) \end{aligned} \quad (15)$$

The exchange of power between the element and its environment takes place in the port at the spatial boundary of the element.

The variables defined around the power conserving structure are the 1-forms  $\phi_1$  and  $e_2$ , and the 0-forms  $\phi_2$  and  $e_1$ . Let us define the following approximation of the one-forms  $\phi_1$  and  $e_2$  :

$$\begin{cases} \bar{\phi}_1(t, r) = \phi_1^{ab}(t) \omega_1^{ab}(r) \\ \bar{e}_2(t, r) = e_2^{ab}(t) \omega_2^{ab}(r) \end{cases} \quad (16)$$

where  $\omega_1^{ab}(r)$  and  $\omega_2^{ab}(r)$  are one-forms satisfying:

$$\int_a^b \omega_i^{ab} = 1 \quad \text{for } i = 1, 2 \quad (17)$$

The 0-forms  $\phi_2$  and  $e_1$  are approximated by:

$$\begin{cases} \bar{e}_1(t, r) = e_1^a(t) \omega_1^a(r) + e_1^b(t) \omega_1^b(r) \\ \bar{\phi}_2(t, r) = \phi_2^a(t) \omega_2^a(r) + \phi_2^b(t) \omega_2^b(r) \end{cases} \quad (18)$$

where the 0-forms satisfy :

$$\begin{aligned} \omega_i^a(a) &= 1, & \omega_i^a(b) &= 0, \\ \omega_i^b(a) &= 0, & \omega_i^b(b) &= 1, \quad \text{for } i = 1, 2 \end{aligned} \quad (19)$$

in order to satisfy to the boundary conditions (15).

##### 4.2 The discretization of the power conserving structure

In the following, we propose to discretize the power conserving structure depicted at the center of the figure Fig.2. Let us first recall the constitutive relation of the conservative structure defined in (11) and associated with the exterior derivative :

$$\begin{cases} \phi_1 = d\phi_2 \\ e_2 = de_1 \end{cases} \quad \begin{cases} e|_{\partial} = e_1|_{\partial\mathcal{R}} \\ \phi|_{\partial} = -\phi_2|_{\partial\mathcal{R}} \end{cases} \quad (20)$$

The approximations of equalities in (20) gives:

$$\bar{\phi}_1 = d\bar{\phi}_2 \quad \bar{e}_2 = d\bar{e}_1 \quad (21)$$

$$\bar{e}|_{\partial} = \bar{e}_1|_{\partial\mathcal{R}} \quad \bar{\phi}|_{\partial} = -\bar{\phi}_2|_{\partial\mathcal{R}} \quad (22)$$

Now let us introduce the approximation formulas (16) and (18) in (21) and integrate along the interval  $[a, b]$  the resulting equations. Thank to (17) and (19) the following equations summarizing the discretized interconnection are obtained:

$$\begin{bmatrix} e_{\partial}^a \\ e_{\partial}^b \\ \phi_{\partial}^a \\ \phi_{\partial}^b \\ \phi_1^{ab} \\ e_2^{ab} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 1 \\ -1 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} e_1^a \\ e_1^b \\ \phi_2^a \\ \phi_2^b \end{bmatrix} \quad (23)$$

Moreover it implies some choice for the forms of the approximations:

$$\begin{aligned} d\omega_2^a(r) &= -\omega_1^{ab}(r) & d\omega_2^b(r) &= \omega_1^{ab}(r) \\ d\omega_1^a(r) &= -\omega_2^{ab}(r) & d\omega_1^b(r) &= \omega_2^{ab}(r) \end{aligned} \quad (24)$$

In order to insure the power conservation of the structure we have to define the internal approximation variables  $\phi_2^{ab}(t)$  and  $e_1^{ab}(t)$  such that the approximated power relation be expressed in the following way:

$$\begin{aligned} P_{ab}(t) &= \int_{ab} \phi_1^{ab}(t) e_1^{ab}(t) + \\ & \int_{ab} \phi_2^{ab}(t) e_2^{ab}(t) + [e_{\partial}(b) \phi_{\partial}(b) - e_{\partial}(a) \phi_{\partial}(a)] \end{aligned} \quad (25)$$

After computation, the approximated power is given by:

$$\bar{P}_{ab}(t) = (\bar{e}_1(b) \bar{\phi}_2(b) - \bar{e}_1(a) \bar{\phi}_2(a)) + [\bar{e}_{\partial}(b) \bar{\phi}_{\partial}(b) - \bar{e}_{\partial}(a) \bar{\phi}_{\partial}(a)] \quad (26)$$

With relations given in (25) and (26), it appears that a general choice for the internal variables can be proposed :

$$e_1^{ab} = \alpha_{ab} e_1^a + \beta_{ab} e_1^b \quad \phi_2^{ab} = \gamma_{ab} \phi_2^a + \delta_{ab} \phi_2^b \quad (27)$$

Taking into account the two last relations of (23), it appears that  $\alpha_{ab} + \beta_{ab} = 1$ ,  $\gamma_{ab} = \beta_{ab}$  and  $\delta_{ab} =$

$\alpha_{ab}$ . In order to obtain a balanced discretization, we will choose for simulation results  $\alpha_{ab} = \frac{1}{2}$ .

The elimination of  $e_1^a$ ,  $e_1^b$ ,  $\phi_2^a$  and  $\phi_2^b$  thank to (23) and (27), the use of (22) and the fact that  $\beta_{ab} = 1 - \alpha_{ab}$  permits to write :

$$\begin{bmatrix} e_1^a \\ e_1^b \\ \phi_2^a \\ \phi_2^b \end{bmatrix} = \begin{bmatrix} 0 & \alpha_{ab} - 1 & 1 & 0 \\ 0 & \alpha_{ab} & 1 & 0 \\ -\alpha_{ab} & 0 & 0 & 1 \\ 1 - \alpha_{ab} & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \phi_1^{ab} \\ e_2^{ab} \\ e_1^{ab} \\ \phi_2^{ab} \end{bmatrix}, \quad \begin{bmatrix} e_\partial^a \\ e_\partial^b \\ -\phi_\partial^a \\ -\phi_\partial^b \end{bmatrix} = \begin{bmatrix} e_1^a \\ e_1^b \\ \phi_2^a \\ \phi_2^b \end{bmatrix} \quad (28)$$

One can show that the previous approximation of the initial power conserving structure remains power conserving. This discretized power conserving structure gives the expression of the boundary variables in function of the discretized internal port variables.

#### 4.3 The discretization of thermodynamical properties

We focus our attention on the right hand side of the figure Fig. 2 relative to the dissipation. Since the linear concentration  $q^L$  belongs to the same space as the flow  $\phi_1$  (a 1-form on the spatial domain), its approximation has to be chosen as :

$$\bar{q}^L(t, r) = -\Psi_1^{ab}(t)\omega_1^{ab}(r) = n^{ab}(t)\omega_1^{ab}(r) \quad (29)$$

with

$$\frac{d\Psi_1^{ab}(t)}{dt} = \phi_1^{ab}(t) = -\dot{n}^{ab}(t) \quad (30)$$

The energy on the element [a,b] is defined as :  $H_C = \int_0^t (\int_{ab} \dot{q}^L(t, r)\mu(t, r)) dt$ . Equation (9) gives the thermodynamical law in the adsorbed scale.

Using the approximation and integrating along the interval [a, b], the approximated energy on the considered volume of micropore is given by :

$$\bar{H}_C = \int_0^t \dot{n}^{ab}(t) \left( \mu^0(T, P_0) + RT \ln \left( \frac{n^{ab}(t)}{P_0 k (n_s^{ab} - n^{ab}(t))} \right) \right) dt$$

Taking into account the expression of the approximated effort  $\bar{e}_C(t, r)$ , which is a 0-form, one obtains the following constitutive relation for the chemical potential internal variable :

$$e_1^{ab} = \mu^0(T, P_0) + RT \ln \left( \frac{n^{ab}(t)}{P_0 k (n_s^{ab} - n^{ab}(t))} \right)$$

Finally we obtain a relation for  $\bar{H}_C$  which is consistent with the fundamental relations of the thermodynamics :

$$e_1^{ab} = \frac{\partial \bar{H}_C}{\partial n^{ab}}. \quad (31)$$

#### 4.4 The discretization of the diffusion equations

The discretized constitutive relation defining the flux due to diffusion may be obtained in an analogous way. Consider the power associated with the diffusion in the microporous medium :

$$P_R = \int_{ab} e_R \phi_R$$

and compute its expression in the discretized variables :

$$\bar{P}_R = \int_{ab} \bar{e}_R \bar{\phi}_R = -\frac{K_{ab}D}{RT} n^{ab}(t) (e_2^{ab}(t))^2$$

with  $K_{ab} = \int_{ab} * \omega_1^{ab}(r) * \omega_2^{ab}(r) \omega_2^{ab}(r)$ .  $q^L(t, r)$  having been approximated by  $\bar{q}^L(t, r) = n^{ab}(t)\omega_1^{ab}(r)$  one can deduce, by identification of the power variables, the discretized flux  $\phi_2^{ab}$  :

$$\phi_2^{ab} = \frac{\partial \bar{P}_R}{\partial e_2^{ab}} = -R_{ab} e_2^{ab}(t) \quad (32)$$

with  $R_{ab}(n^{ab}) = \frac{2K_{ab}D}{RT} n^{ab}$ .

## 5. SIMULATION RESULTS

In order to satisfy the condition (17), the one-forms  $\omega_i^{ab}$  are defined by  $\omega_i^{ab} = \frac{dz}{b-a}$ . The zero-forms  $\omega_i^a$  and  $\omega_i^b$  are defined such that Eq. (15) is satisfied. So we have  $\omega_i^a = \frac{b-r}{b-a}$ ,  $\omega_i^b = \frac{r-a}{b-a}$ . The spatial domains (all the scales are considered for simulation) are discretized in equal meshes in each scale (10 meshes for each scale). The discretized model is simulated with the physical parameters presented in (Jolimaitre, 1999).

This simulation is performed for a separation of mixture of two constituents,  $O_2$  and  $N_2$ . The simulated experiment is the response of an adsorption column, initially saturated in  $N_2$  to a steam of air. The process is initially at equilibrium which corresponds to  $\mu = 0$  all along the profile (in each point in the simulated column).

In Fig. 3-a, the output of the column is initially saturated with  $N_2$  is shown. In Fig. 3-b, the concentration of the first constituent at the first, sixth and last mesh of the extragranular phase is represented. In Fig.3-c, the concentrations in the macroporous medium attached to the last discretized mesh of the column is given. The curves correspond to the first, the sixth and the last mesh. In Fig.3-d, the concentration in the microporous medium attached at boundaries of the pellet (the last mesh) which is itself attached in the last mesh of the column.

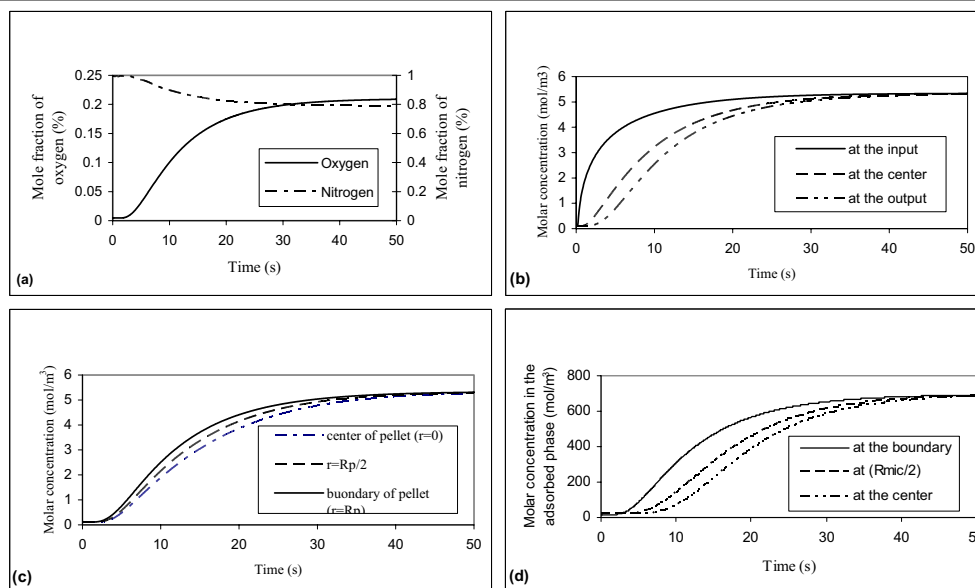


Fig. 3. Simulation results

## 6. CONCLUSION

In this paper we discussed the port-based modelling and spatial discretization of distributed parameter systems. In order to illustrate this approach, a model of adsorption column has been derived directly from its thermodynamical description. The modelling methodology presented exhibits some interesting features :

- The modelling is coordinate free.
- The model is a network model where each element represents a specific phenomenon which may be identified from a thermodynamics point of view.
- The instantaneous power conservation and the description of the power transfers within the system and through its boundaries are explicitly represented.

These properties of the model have several important consequences :

- The derived model requires parameters that have a clear physical meaning. This considerably simplifies the parameters estimation task.
- The model is acausal, hence postpones the choice of boundary conditions (for instance depending here on the model of the gaseous phase in the adsorption column) and is thus clearly reusable.
- The central geometric Dirac structure is a direct generalization of Poisson structure in Hamiltonian systems. It suggests and allows the use of passivity-based or energy-shaping techniques for control purposes.

These considerations strongly encourage the development of a discretization method which pre-

serves both the nature of the interconnection structures and the physical properties of the connected elements. Such a method has been presented in this paper. Its numerical effectiveness has been established. But the key point is that we now possess a reduced model which allows a direct use of the geometric and thermodynamics properties of the PDEs model to develop estimation or control algorithms. Both the model and the discretization method apply for a large class of distributed parameters thermodynamics systems.

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