Structure-preserving collocation method
for parabolic systems
Application to a diffusion Process.

F.Couenne   B. Hamroun

*Univ Lyon, Université Claude Bernard Lyon 1, CNRS UMR 5007,
LAGEP F-69622, LYON, FRANCE (e-mails:
{couenne;hamroun}@lagep.univ-lyon1.fr).*

Abstract: In this contribution we present the reduced port Hamiltonian model of a parabolic system obtained by a structure preserving collocation method. It is applied to a nonlinear diffusion process involving two species in gas phase at constant pressure and temperature.

Keywords: port Hamiltonian modeling, model reduction, infinite dimensional systems, transport phenomena

1. INTRODUCTION

Spatial reduction is an important concern for simulation and control of distributed parameter systems. Besides traditional spatial discretization methods such finite difference methods or weighted residual methods (Villadsen and Michelsen, 1978) there exist methods that preserve the port Hamiltonian structure of the original systems such mixed finite elements methods (Bossavit, 1998; Golo et al., 2004; Baaiu et al., 2009) that have been applied to hyperbolic and parabolic systems and pseudo spectral methods applied to hyperbolic systems (Moulla et al., 2012). This paper is intended to present the discretization thanks to the structure preserving collocation method presented in (Moulla et al., 2012) of a parabolic system : a two constituent diffusion process in gas phase at constant pressure and temperature. A very similar idea is developed in Vu et al. (2013) on the resistive diffusion equation (which is basically a diffusion equation).

The port Hamiltonian formulation of distributed parameter systems is based on the generalization of the finite dimensional Dirac structure (Courant, 1990; Dorfman, 1993). This geometrical structure relates the flow and effort variables through a skew symmetric operator which interprets the power conservation principle. In (Moulla et al., 2012), the authors propose the discretisation of the Dirac structure of hyperbolic systems as well as the discretization of the constitutive equation (which can be nonlinear) of the Hamiltonian for the case of lossless systems with two domains of energy. In the case of a diffusion process in order to obtain a Stokes-Dirac structure we have to extend the vector of port variables with the resistive port variables. The considered case deals with one domain of energy: the material domain.

So in this paper we present the discretisation of the extended Dirac structure, the discretisation of the Hamiltonian as well as the discretization of the dissipation law.

2. STRUCTURED MODELLING OF THE DIFFUSION SYSTEM

In this section we present the port based modelling approach for diffusion in a capillary of a zeolite. Zeolites are microporous, aluminosilicate minerals commonly used as adsorbents and catalysts. In this paper, we consider the diffusive transport of two constituents within the pores of zeolite: a capillary.

2.1 Model of the diffusion in a capillary of a zeolite

Diffusion of the two constituents inside the cylindrical capillary is expressed in terms of Stefan Maxwell law (Krishna and J.A.Wesselingh, 1997). The cylindrical capillary is considered with length L and constant section. The gas mixture is assumed to be ideal. The temperature T and pressure P inside the capillary are assumed to be constant. So thanks to the perfect gas law, the total mole concentration c_t present in the capillary is constant. Cylindrical symmetries are assumed for the mole and energy balances.

As a consequence, the standard material balance for the species i over the spatial domain $X = [0, L]$ is given by:

$$\int_X \frac{\partial}{\partial t} c_i dx = - \int_X \frac{\partial J_i}{\partial x} dx \qquad (1)$$

where $c_i(x, t)$ is the lineic mole concentration of speciies i, $J_i = -\frac{D_d x_i}{RT} \frac{\partial \mu_i}{\partial x}$ is the lineic diffusion flux density, R is the perfect gas contant, μ_i is the chemical potential of the constituent i, x_i the mole fraction of constituent i and D_d the diffusion constant.

Since the proposed discretization method aims at preserving the structure associated with both material and energy balances, the choice of the manipulated variables concerns moles and energy. The system being isothermal and isobaric, Gibbs free energy can be considered instead of internal energy. From thermodynamic considerations (Callen, 1985), we finally obtain the Gibbs free energy balance:

$$\frac{\partial}{\partial t} \int_X g dx = - \int_X \sum_i \frac{\partial g}{\partial c_i} \frac{\partial c_i}{\partial t} dx = - \int_X \sum_i \mu_i \frac{\partial c_i}{\partial t} dx \tag{2}$$

where g is the lineic density of the free Gibbs energy lineic density (J/m).

2.2 Port-based model of the diffusion in a capillary of a zeolite

From now, we will consider exterior differential forms (Flanders, 1989) in order to discriminate between the different variables. Two kinds of variables appear in model the 0-forms and the 1-forms. We will denote $\Lambda^0(X)$, $\Lambda^1(X)$ the spaces of the 0-forms on the interval $[0, L]$ and of the 1-forms on the interval $[0, L]$, respectively. The balance equation (1) can be rewritten as:

$$\int_X \frac{\partial c_i}{\partial t} = - \int_X dJ_i \tag{3}$$

where d is the exterior derivative that will represent indifferently divergence or gradient, c_i, $\frac{\partial c_i}{\partial t}$, dJ_i are 1-forms that can be evaluated on any interval included in X , i.e. $c_i, dJ_i \in \Lambda^1(X)$, and $J_i \in \Lambda^0(X)$ is a 0-form that can be evaluated at any point of X.

In a same way we have $g \in \Lambda^1(X)$ with its balance equation rewritten as follows:

$$\int_X \frac{\partial}{\partial t} g = \int_X \sum_i \mu_i \frac{\partial c_i}{\partial t} \tag{4}$$

Replacing $\frac{\partial c_i}{\partial t}$ by its expression in (3) and applying the Stokes theorem, the time derivative of the Gibbs free energy can be written:

$$\frac{d}{dt} \int_X g = \int_X \sum_i \mu_i^T (-dJ_i)$$
$$= - \int_{\partial X} \sum_i \mu_i^T J_i + \int_X \sum_i d(\mu_i)^T J_i \tag{5}$$

The relation (5) shows the natural choice of the effort and flow variables on which the geometric Stokes Dirac structure (see (Schaft and B.Maschke, 2002)) of the port based formulation will be defined.

The chosen variables for the structured modeling are the following:

- The 1-forms $\begin{pmatrix} f_i \\ e_{Ri} \end{pmatrix} = \begin{pmatrix} dJ_i \\ d\mu_i \end{pmatrix}$ are made up with the flow density and the chemical potential gradient.
- The 0-forms $\begin{pmatrix} e_i \\ f_{Ri} \end{pmatrix} = \begin{pmatrix} \mu_i \\ J_i \end{pmatrix}$ are made up with the chemical potential and the flux density.

Where (f_i, e_i) and (f_{Ri}, e_{Ri}) are the couples of power conjugated effort and flow variables. The boundary power conjugated port variables $(f_{\partial i}, e_{\partial i})$ can be defined as a linear combination of the boundary conditions $\mu_i(0, t)$, $\mu_i(L, t)$, $J_i(0, t)$ and $J_i(L, t) \in \Lambda^0(\partial X)$ such that Stoke's theorem (5) is satisfied (Gorrec et al. (2005)):

$$\sum_i \left(\int_X e_i^T f_i + \int_X e_{Ri}^T f_{Ri} \right) + \sum_i e_{\partial i}^T f_{\partial i} = 0 \tag{6}$$

For simplicity let us choose:

The quadruple $\left(\begin{pmatrix} f_1 \\ e_{R1} \\ f_2 \\ e_{R2} \end{pmatrix}, \begin{pmatrix} f_{\partial 1} \\ f_{\partial 2} \end{pmatrix}, \begin{pmatrix} e_1 \\ f_{R1} \\ e_2 \\ f_{R2} \end{pmatrix}, \begin{pmatrix} e_{\partial 1} \\ e_{\partial 2} \end{pmatrix} \right)$

such that the port based formulation of diffusion of these two species is given by:

$$\begin{pmatrix} f_1 \\ e_{R1} \\ f_2 \\ e_{R2} \end{pmatrix} = \begin{pmatrix} 0 & d & 0 & 0 \\ d & 0 & 0 & 0 \\ 0 & 0 & 0 & d \\ 0 & 0 & d & 0 \end{pmatrix} \begin{pmatrix} e_1 \\ f_{R1} \\ e_2 \\ f_{R2} \end{pmatrix} \tag{7}$$

and

$$\begin{pmatrix} f_{\partial 1} \\ f_{\partial 2} \\ e_{\partial 1} \\ e_{\partial 2} \end{pmatrix} = \begin{pmatrix} \begin{bmatrix} -f_{R1}(L) \\ f_{R1}(0) \\ -f_{R2}(L) \\ f_{R2}(0) \end{bmatrix} \\ \begin{bmatrix} e_1(L) \\ e_1(0) \\ e_2(L) \\ e_2(0) \end{bmatrix} \end{pmatrix} \tag{8}$$

defines a Stokes Dirac structure $\mathcal{D}$ (Schaft and B.Maschke, 2002) for the bilinear product (6).

This geometric power preserving structure has to be completed with two closure equations for the effort variables e_i and flow variables f_{Ri}:

- The computation of the effort variables e_i corresponding to chemical potential of an ideal mixture is written as a function of c_i expressed as: $e_i = \mu_i = \mu_{0i} + RTlog(\frac{*c_i}{c_t})$ where * is the Hodge star operator and $*c_i \in \Lambda^0(X)$
- The computation of the flow variables f_{Ri} is done from the Stefan Maxwell diffusion law: $J_i = -\frac{D_d *c_i}{RTc_t} * de_i$ where $e_i = \mu_i \in \Lambda^0(X)$, $de_i = d\mu_i \in \Lambda^1(X)$, $* de_i = *d\mu_i \in \Lambda^0(X)$.

In the next section we present the geometrical reduction of the diffusion process.

3. MODEL REDUCTION BASED ON GEOMETRICAL PROPERTIES

We follow the method proposed in (Moulla et al., 2012). For simplicity, we present the method for only one constituent so we omit the index of the constituent. The approximation method is based on the separation of variables method. The chosen approximation bases are different according to the degree of the considered differential forms. The 0-form variables e and f_R are approximated on X by:

$$\begin{cases} \overline{e}(t, x) = \sum_{i=0}^N e_i(t) \phi_i(x) & , e_i \in \mathbb{R} \\ \overline{f_R}(t, x) = \sum_{i=0}^N f_{Ri}(t) \phi_i(x) & , f_{Ri} \in \mathbb{R} \end{cases} \tag{9}$$

The 1-form variables f and e_R are approximated on X by:

$$\begin{cases} \overline{f}(t, x) = \sum_{j=1}^N f_j(t) \psi_j(x) dx & , f_j \in \mathbb{R} \\ \overline{e_R}(t, x) = \sum_{j=1}^N e_{Rj}(t) \psi_j(x) dx & , e_{Rj} \in \mathbb{R} \end{cases} \tag{10}$$