Energy-preserving method for spatial discretization: application to an adsorption column.

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Abstract

This paper deals with the spatial discretization of distributed parameter systems. The originality of the proposed approach is to combine geometrical modelling and finite element discretization method to preserve the model structure associated with both mass and energy balances during the spatial reduction. The approach is presented through the example of an adsorption process. The methodology is described on the microporous phase.

Keywords: spatial discretization, infinite dimensional systems, adsorption process, thermodynamic systems, port-based modeling.

1. Introduction

The aim of this paper is to present a method for spatial discretization of distributed parameters systems. The originality of this work is the use of Port Based Modeling (PBM) approach for both process modeling and discretization (Karnopp 2000). Let us recall that the power of PBM is that interconnection is done in a natural way as soon as port variables are chosen as power conjugate variables like in thermodynamics (De Groot and Mazur 1984). Moreover, models of systems are manipulated as a set of interconnected and reusable sub-models whose basic elements are accumulation element, dissipation element and power preserving interconnection structure.

The structure issued from PBM (see for instance Couenne et al. (2006), Couenne et al. (2007)) is used in order to characterize the energetic behavior of the system and as a basis of our discretization mixed finite element method. The final goal of this method is by an appropriate choice of power conjugate variables to preserve during the discretization stage the energy balances as well as the structural properties of the distributed model in terms of energy. In this way the method guarantees the easy interconnection of the discretized model (Couenne et al. 2007) and its reusability.

This preservation of structure is important for control purpose since we now possess a reduced model which allows a direct use of the geometric and thermodynamics properties of the PDEs model to develop control algorithms. As an example, passivity based or energy-shaping techniques can be applied (Ortega et al. 2002) for stabilization and regulation purposes on such a model.

As an example we will treat the case of an adsorption column with bidisperse pellets based on Maxwell Stefan formulation of diffusion (Krishna 1990). The column is mathematically described by a set of interconnected Partial Differential Equations (PDE's). Traditional modeling of such system does not take into account any structure of the constitutive equations and the choice of the state variables can lead to numerical difficulties, especially during the interconnection of the different levels. The partial

model (microporous phase) is presented in Couenne et al. (2005). The complete port based model of the column is given in Baaiu et al (2006). In this paper we focuse to the microporous phase modeling and discretization. The modelling and reduction of the other phases will be obtained with the same methodology as it will be seen.

2. Basis of the structured modelling of an adsorption column

Let first recall all the assumptions we made over the entire column:
1. We consider an ideal binary mixture constituted of an inert gas and one component that can be adsorbed.
2. The adsorption column is supposed to be at constant temperature and pressure. The velocity v of the flowing fluid is also supposed to be constant.
3. The diffusion onto the surface of the crystal and the diffusion into the macropore volume are represented by using the Knudsen/Maxwell-Stefan formulation (Krishna 1997) . This choice is adequate since flux is expressed thanks to the thermodynamic chemical potential. The Langmuir model for the adsorption equilibrium is used.
4. In the extragranular phase, a dispersion phenomenon is taken into account. It is represented with a constant axial dispersion coefficient D.
5. The column is supposed to be cylindrical with constant cross section. The particles and the crystals are supposed to be spherical with uniform radius. Spherical symmetries are supposed both in the macropore phase and in the adsorbent.

As mentioned modelling and discretization methods have been applied to the each phase of the column. From the assumptions each level leads to a 1D model. Let us now review in details the port based model for the microporous scale only. Remarks about the other phases will be made along the section.

2.1. Modelling of the microporous scale

From a mathematical point of view, we use the framework of differential geometry (Flanders 1989) to obtain a coordinate free model of the considered process. In this framework d is the exterior derivative (in the general case it is the div or gradient; in catesian 1D it reduces to $\dfrac{\partial}{\partial r}$). The general balance equation for species i is given by:

$$\int_{\Omega} \frac{\partial q_i}{\partial t} = \int_{\Omega} d(-N_i) \tag{1}$$

With the concentration q_i, the diffusive molar flux N_i. Ω represents the 1D domain $[0, R]$, R being the mean radius of the crystals. Since the proposed discretization method must preserve the structure associated with both mass and energy balances, the choice of the manipulated variables must concern mass and energy. In order to obtain the right power conjugate variables, let us write the (Gibbs free) energy density g balance:

$$\frac{d}{dt} \int_{\Omega} g = \int_{\Omega} \sum_i d(-N_i) \mu_i \tag{2}$$

with $\mu_i = \dfrac{\partial g}{\partial q}$ the chemical potential of species *i*. Applying Stoke's theorem to equation (2), its finally results (Couenne et al. 2005):

$$\int_{\partial\Omega} \mu^T N = \int_{\Omega} d\mu^T\, N + \int_{\Omega} \mu^T\, dN \tag{3}$$

with standard vectorial notation. $\partial\Omega = \{0, R\}$ and $d\mu$ corresponds to $grad\ \mu$. Equation (3) expresses the power continuity between internal power variation and the power flow at boundaries. Moreover it imposes the choice of the manipulated power conjugate variables (μ, dN) and $(d\mu, N)$. It makes appear the geometric structure representative of the infinite dimensional mass balance,

$$\begin{pmatrix} dN \\ d\mu \end{pmatrix} = \begin{pmatrix} 0 & d \\ d & 0 \end{pmatrix}\begin{pmatrix} \mu \\ N \end{pmatrix} \tag{4}$$

which is with the appropriate boundary pairing $(\mu \quad N)\big|_0$ and $(\mu \quad N)\big|_R$ a Dirac structure (Maschke and van der Schaft 2004).

The originality of our approach is to use this geometric power conserving structure for the modelling of dissipative systems. This is the price to pay to interconnect easily systems (Maschke and van der Schaft 2004). To summarize, the aforementioned power preserving structure represents the interconnection between the storage, dissipative and boundary parts of the model. It combines two adjoint differential relations, namely the generating force as the gradient of the chemical potential and the conservation law (1) by the divergence of the flux. Moreover it is the central element of the structured modelling of mass transport phenomena. It will appear at each phase of the model.

This model has to be completed with two closure equations between effort and flux variables related with accumulation and dissipation terms. The resulting structured model is depicted on Figure1. This model is valid for the microporous level but also for the other level.

The element $\mathscr{C}$ is related to the accumulation and represents the left hand side of equation (1). q can be computed from dN and F_{distr} by time integration (this is done to homogeneous μ thank to the local equilibrium thermodynamic condition) and μ from q using the thermodynamic constitutive equation (first closure equation).

Remark: In the case of the microporous phase, the distributed flow $F_{distr} = 0$. It is not the case for the other levels. For example, in the extragranular level, F_{distr} corresponds to the total flow coming from all the crystals present in the macroporous sub domain.
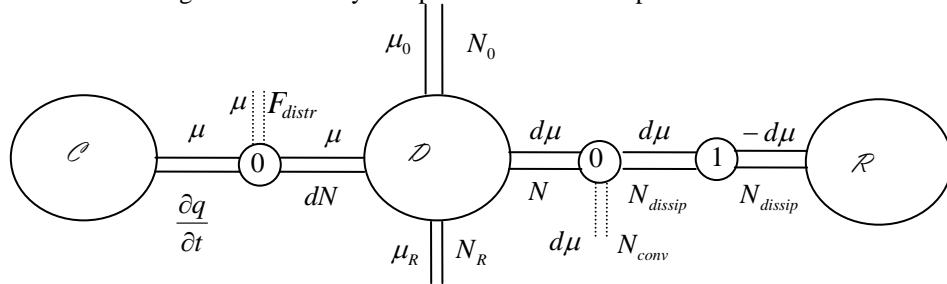
Fig 1: Structured representation of the transport phenomena.

The element $\mathcal{R}$ is related to the dissipation (diffusion or dispersion). The flux N_{dissip} is computed from the driving force $-d\mu$ using the second phenomenological law. The element $\mathcal{D}$ is the power preserving structure described by equation (4). The power continuous junctions 0 and 1 express the continuity of flow variables (extensive variables) and effort (intensive variables) respectively.

Remark: It can be seen that in the extragranular phase the convective flux N_{conv} has be added between the elements $\mathcal{D}$ and $\mathcal{R}$ ($N = N_{dissip} + N_{conv}$).

2.2. Interconnection of the level
The assumption for the interconnection of phases is that the crystal repartition into the pellets is uniform as well as the pellet repartition within the column. Furthermore all the boundaries of the considered level are at local equilibrium with variables of the upper level. Considering spherical symmetry, the crystals have the same chemical potential than the pellet. This means that there is an equality of efforts at the boundary. Continuity of flux at the boundary of the crystal is also considered. As a consequence, the flux coming from all the crystals present in the sub domain can be seen as a distributed source of flux for the pellet. It can be shown that these relations define a power continuous coupling between the levels (Couenne et al. 2005).

3. Model reduction based on geometrical properties
The proposed discretization method consists in splitting the initial structured infinite dimensional model into n finite dimensional sub-models (finite elements) with the same energetic behavior. Structure given in figure 1 is still enforced.

3.1. Approximation of forms
For this purpose we consider the local domain $R_{ab} = [a,b] \subset [0,R]$. 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. From the observation of equation (4), μ and N are functions (0-form) since they can be evaluated at any point of Ω whereas $d\mu$ and dN are 1-forms since they can be evaluated by integration along Ω. For simplicity let us set $\mu_d = d\mu$ and $N_d = dN$.

The 1-forms are approximated on R_{ab} by $\overline{\mu_d}(r,t) = \mu_d^{ab}(t)\omega_{\mu_d}^{ab}(r)$ and $\overline{N_d}(r,t) = N_d^{ab}(t)\omega_{N_d}^{ab}(r)$ where the support 1-forms $\omega_{\mu_d}^{ab}(r)$ and $\omega_{N_d}^{ab}(r)$ are chosen such that $\int_{R_{ab}} \omega_{\mu_d}^{ab} = \int_{R_{ab}} \omega_{N_d}^{ab} = 1$ which implies that $\mu_d^{ab}(t) = \int_{R_{ab}} \overline{\mu_d}(t,r)$ and $N_d^{ab}(t) = \int_{R_{ab}} \overline{N_d}(t,r)$. The 0-form μ and N are approximated on R_{ab} by:

$$\overline{\mu}(r,t) = \mu(a,t)\omega_\mu^a(r) + \mu(b,t)\omega_\mu^b(r) \quad \overline{N}(r,t) = N(a,t)\omega_N^a(r) + \mu(b,t)\omega_N^b(r)$$

where the support 0-forms are chosen such that:

$$\omega_\mu^a(a) = \omega_\mu^b(b) = 1, \ \omega_\mu^a(b) = \omega_\mu^b(a) = 0, \omega_N^a(a) = \omega_N^b(b) = 1, \ \omega_N^a(b) = \omega_N^b(a) = 0$$

This choice is done such that $\overline{\mu}(a,t) = \mu(a,t)$ and $\overline{\mu}(b,t) = \mu(b,t)$. For simplicity we choose the same support 0-forms ω^a and ω^b for $\overline{\mu}$ and $\overline{N}$ and the same support 1-form ω^{ab} for $\overline{\mu_d}$ and $\overline{N_d}$.

3.2. Discretization of the interconnection structure

The interconnection structure of each submodel is finite dimensional and concerns the reduced variables $\overline{N_d}$ and $\overline{\mu_d}$ and their power conjugate variables $\overline{\mu}$ and $\overline{N}$. In order to have a finite dimensional power preserving structure, the reduced variables have to satisfy (Golo et al. 2004):

$$E\begin{pmatrix} \mu^{ab} & N^{ab} & \mu_\partial^a & \mu_\partial^b \end{pmatrix}^T + F\begin{pmatrix} \mu_d^{ab} & N_d^{ab} & N_\partial^a & N_\partial^b \end{pmatrix}^T = 0 \tag{5}$$

with $\begin{bmatrix} E & F \end{bmatrix}$ full rank and $EF^T + FE^T = 0$.

For this purpose, we require that the approximation variables satisfy the relation induced by the interconnection structure (4). It leads to the following relations between the approximated variables with $\alpha_{ab} = \int_{R_{ab}} \omega^b \omega^{ab}$:

$$\begin{cases} N_d^{ab} = N(b) - N(a) = N_\partial^b - N_\partial^a \\ \mu_d^{ab} = \mu(b) - \mu(a) = \mu_\partial^b - \mu_\partial^a \end{cases} \tag{6}$$

and

$$\begin{cases} N^{ab} = (1 - \alpha_{ab})N(a) + \alpha_{ab}N(b) = (1 - \alpha_{ab})N_\partial^a + \alpha_{ab}N_\partial^b \\ \mu^{ab} = (1 - \alpha_{ab})\mu(b) + \alpha_{ab}\mu(a) = (1 - \alpha_{ab})\mu_\partial^b + \alpha_{ab}\mu_\partial^a \end{cases} \tag{7}$$

Equations (7) are obtained from the net power expressed with approximate variables. We have 8 variables and 4 equations but two are input variables. So we have to characterize two relations consisting in the discretized version of the constitutive relations.

3.3. Discretization of the diffusion equation

The purpose of this section is to compute N^{ab} from the driving force such that energy structure of the element $\mathcal{R}$ is preserved: $\overline{G_R^{ab}} = \mu_d^{ab} N^{ab} = \int_{R_{ab}} \overline{\mu_d} \overline{N}$.

The diffusion represented by Knudsen law can be written as $N = -\dfrac{D*q}{RT}*\mu_d$. For a 1-form f on 1D domain, it can be written $f = \dfrac{\partial f}{\partial r}dr$ and the Hodge star operator *

represents the function $* f = \dfrac{\partial f}{\partial r}$. Writing the instantaneous power of this element with

approximate variables and after identification $N^{ab} = \dfrac{\partial G_R^{ab}}{\partial \mu_d^{ab}} = -2K^{ab}R\mu_d^{ab}$ with

$K^{ab} = \displaystyle\int_{R_{ab}} \omega^{ab} * \omega^{ab}$ depending on support forms and $R = \dfrac{D*q}{RT}$.

3.4. Discretization of the accumulation

The principle is the same than for the $\mathscr{R}$ element. The purpose is to compute μ^{ab} from

q . The approximate energy on R_{ab} of the $\mathscr{C}$ element is $\overline{G_C^{ab}} = \displaystyle\int_{R_{ab}} \overline{\dot{q}}\overline{\mu}$. Let us note that

the linear concentration q lies in the same space than the flow variable $\dot{q}$ as well as the

linear saturation concentration q_s appearing in the Langmuir model so the same support

function can be used. We finally obtain for the discretized chemical potential

$$\mu^{ab}(t) =: \frac{\partial \overline{G_C^{ab}}}{\partial q^{ab}} = \mu^{ref}(T,P) + RT\ln(\frac{1}{P}\frac{q^{ab}}{k(q_s^{ab}-q^{ab})})$$

Using the same procedure, the other level are also discretized. Mainly only constitutive relations of accumulation and dissipation are changed. Finally the coupling of the different levels is performed.

4. Conclusion

In this paper we present a discretization method which preserves both the nature of the interconnection structures and the physical properties of the connected elements.

We apply this method with the simplest support forms $\omega^{ab} = \dfrac{1}{b-a}dr$,

$\omega^a = \dfrac{b-r}{b-a}$ and $\omega^b = \dfrac{r-a}{b-a}$. Numerical results are presented in (Baaiu 2006).

This choice of forms leads to a centered method. The quality of numerical results can be compared advantageously to those obtained with a left finite difference method.

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