BG-CFD Methodology for Multicomponent Solutions. Part I: Multivelocity Model

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Abstract— **This paper shows an application to Multicomponent Solutions of a new, Bond-Graph based formalism for CFD problems. It is shown that, for the multivelocity model, the resulting independent variables are the densities and velocities of the components and the entropy per unit volume. The state equations are derived, showing the potentials and constitutive relations needed to describe a multicomponent system.**

Keywords: **Bond Graphs, Computational Fluid Dynamics, CFD, Multicomponent Solutions.**

I. INTRODUCTION

In recent works [1][2] a theoretical development of a general Bond Graph approach for CFD was presented. This new methodology, which was called BG-CFD [3], is a result of the right combination of Bond-Graph concepts with elements of numerical methods. In this paper, the methodology described above is extended to multicomponent solution systems.

A classical mixture, or solution, is a material in which the components are not physically distinct, that is, the mixing is at molecular level. In this case, when described using Continuum Theory, all the components of the solutions are able to occupy the same region of space at the same time [4] and can be assumed to be in thermodynamic equilibrium. In a solution, each component has its own velocity, density and internal energy. The balance principles for the constituents resemble those for a single component, except that the constituents are allowed to interact with one another.

Concerning the nomenclature, bold letters will be used to define first order tensors ($\boldsymbol{V}^{(i)}$, $\boldsymbol{p}_v^{(i)}$, etc.). Column vectors associated to nodal values will be denoted by single underscored plain or bold type ($\underline{m}^{(i)}$, $\underline{\boldsymbol{S}}^{(i)}$, $\underline{\boldsymbol{V}}^{(i)}$, $\underline{r}_o^{(i)}$, etc.) while multidimensional matrices will be identified by double underscored plain type (*e.g.* $\underline{\underline{M}}^{(i)}$, $\underline{\underline{\Omega}}_\rho^{(i)}$, etc.). Second order tensors will be denoted by bold, double underscored type (*e.g.* $\underline{\underline{\boldsymbol{\tau}}}^{(i)}$, $\underline{\underline{\mathbf{I}}}$). Einstein convention of summation over repeated indices is *not* used.

II. INDEPENDENT VARIABLES AND POTENTIALS

A. *Internal Energy per Unit Volume*

For a multicomponent solution with r components, the internal energy per unit volume u_v can be written as a function of the entropy per unit volume s_v and the component densities $\rho^{(i)}$:

$$u_v = u_v(s_v, \rho^{(1)}, ..., \rho^{(r)}) \tag{1}$$

The following potentials are defined:

$$\theta = \left(\frac{\partial u_v}{\partial s_v}\right)_{\rho^{(i)}} \quad ; \quad \mu^{(i)} = \left(\frac{\partial u_v}{\partial \rho^{(i)}}\right)_{s_v,\, \rho^{(j\neq i)}} \tag{2}$$

where θ is the temperature and $\mu^{(i)}$ is the ith-species chemical potential per unit mass. The pressure P can be obtained from the Euler equation [5]:

$$u_v = \theta\, s_v - P + \sum_{i=1}^{r} \mu^{(i)}\, \rho^{(i)} \tag{3}$$

The time derivative of the internal energy per unit volume can be written as:

$$\frac{\partial u_v}{\partial t} = \sum_{i=1}^{r} \mu^{(i)} \frac{\partial \rho^{(i)}}{\partial t} + \theta \frac{\partial s_v}{\partial t} \tag{4}$$

An analog description is adopted for the internal energy per unit volume corresponding to the ith-component $u_v^{(i)}$:

$$u_v^{(i)} = u_v^{(i)}(s_v, \rho^{(1)}, ..., \rho^{(r)}) \tag{5}$$

The following potentials are defined:

$$\pi^{(i)} = \left(\frac{\partial u_v^{(i)}}{\partial s_v}\right)_{\rho^{(j)}} \quad ; \quad \mu^{(ij)} = \left(\frac{\partial u_v^{(i)}}{\partial \rho^{(j)}}\right)_{s_v,\, \rho^{(k\neq j)}} \tag{6}$$

where $\pi^{(i)}$ and $\mu^{(ij)}$ can be regarded as ith-component contributions to the temperature and chemical potentials. From the Euler equation:

$$u_v^{(i)} = \pi^{(i)}\, s_v - P^{(i)} - \sum_{j=1}^{r} \mu^{(ij)}\, \rho^{(j)} \tag{7}$$

where $P^{(i)}$ is the ith-component contribution to the pressure. Since:

$$u_v = \sum_{i=1}^{r} u_v^{(i)} \tag{8}$$

the following relations are verified:

$$\theta = \sum_{i=1}^{r} \pi^{(i)} \quad ; \quad \mu^{(i)} = \sum_{j=1}^{r} \mu^{(ji)} \quad ; \quad P = \sum_{i=1}^{r} P^{(i)} \tag{9}$$

As an example, the potentials associated to the entropic representation of the ith-component internal energy are calculated in Section VI for the case of a mixture of ideal gases.

B. *Kinetic Coenergy per Unit Volume*

The kinetic energy per unit volume t_v^* can be written as a function of the component densities and velocities $\boldsymbol{V}^{(i)}$:

$$t_v^* = \sum_{i=1}^{r} \frac{1}{2} \rho^{(i)}\, \boldsymbol{V}^{(i)2} \tag{10}$$

In a companion paper [6], it is presented an approximation in which the dynamics of a multicomponent solution is described in terms of the average (center of mass) velocity of the mixture and the mass flux of each component relative to the average velocity; these relative mass fluxes are modeled using diffusion theory. The following potentials are defined:

$$\kappa^{(i)} = \left(\frac{\partial t_v^*}{\partial \rho^{(i)}}\right)_{\rho^{(j\neq i)},\, \boldsymbol{V}^{(k)}} = \frac{1}{2}\, \boldsymbol{V}^{(i)2} \tag{11}$$

$$\boldsymbol{p}_v^{(i)} = \left(\frac{\partial t_v^*}{\partial \boldsymbol{V}^{(i)}}\right)_{\rho^{(j)},\, \boldsymbol{V}^{(k\neq i)}} = \rho^{(i)}\, \boldsymbol{V}^{(i)} \tag{12}$$

The time derivative of the kinetic coenergy per unit volume can be written as:

$$\frac{\partial t_v^*}{\partial t} = \sum_{i=1}^{r} \left(\kappa^{(i)} \frac{\partial \rho^{(i)}}{\partial t} - \boldsymbol{p}_v^{(i)} \cdot \frac{\partial \boldsymbol{V}^{(i)}}{\partial t}\right) \tag{13}$$

C. *Total Energy per Unit Volume*

The total energy per unit volume e^* includes the internal energy and the kinetic coenergy:

$$e_v^* = u_v + t_v^* \tag{14}$$

The time derivative of the total energy per unit volume can be written as:

$$\frac{\partial e_v^*}{\partial t} = \theta \frac{\partial s_v}{\partial t} - \sum_{i=1}^{r} \left[\left(\mu^{(i)} + \kappa^{(i)} \right) \frac{\partial \rho^{(i)}}{\partial t} + \boldsymbol{p}_v^{(i)} . \frac{\partial \boldsymbol{V}^{(i)}}{\partial t} \right] \tag{15}$$

Since the internal energy and kinetic coenergy are continuous functions of the independent variables, the potentials multiplying the time derivatives of the independent variables satisfy both constitutive and Maxwell relations [5].

III. BALANCE EQUATIONS

The balance equations are power equations corresponding to each one of the terms that contributes to the time derivative of the total energy per unit volume. For multicomponent solutions, the balance equations can be derived from the mass, momentum and energy conservation equation corresponding to each component [4]:

$$\frac{\partial \rho^{(i)}}{\partial t} = -\nabla . \left(\rho^{(i)} \, \boldsymbol{V}^{(i)} \right) + C^{(i)} \tag{16}$$

$$\rho^{(i)} \frac{\partial \boldsymbol{V}^{(i)}}{\partial t} = -\rho^{(i)} \, \boldsymbol{V}^{(i)} . \nabla \boldsymbol{V}^{(i)} + \nabla . \underline{\underline{\boldsymbol{T}^{(i)}}} + \rho^{(i)} \, \boldsymbol{G}^{(i)} + \boldsymbol{f}^{(i)} - C^{(i)} \, \boldsymbol{V}^{(i)} \tag{17}$$

$$\frac{\partial u_v^{(i)}}{\partial t} = -\nabla . \left(u_v^{(i)} \, \boldsymbol{V}^{(i)} \right) - \boldsymbol{f}^{(i)} . \boldsymbol{V}^{(i)} + C^{(i)} \frac{1}{2} \boldsymbol{V}^{(i)2} + \underline{\underline{\boldsymbol{T}^{(i)}}} : \nabla \boldsymbol{V}^{(i)} + \rho^{(i)} \, \Phi^{(i)} - \nabla . \boldsymbol{q}^{(i)} + \epsilon^{(i)} \tag{18}$$

where $C^{(i)}$, $\boldsymbol{f}^{(i)}$ and $\epsilon^{(i)}$ are correspondingly the mass, momentum and energy interaction terms (per unit volume), $\Phi^{(i)}$ is the heat power source per unit mass, $\boldsymbol{G}^{(i)}$ is the body force, $\boldsymbol{q}^{(i)}$ is the heat flux and $\underline{\underline{\boldsymbol{T}^{(i)}}}$ is the stress state for the ith-component.

Since there are no distributional sources, it is postulated that the sum of the interactions of mass, momentum and energy vanish, that is:

$$\sum_{i=1}^{r} C^{(i)} = 0 \;\; ; \;\; \sum_{i=1}^{r} \boldsymbol{f}^{(i)} = \boldsymbol{0} \;\; ; \;\; \sum_{i=1}^{r} \epsilon^{(i)} = 0 \tag{19}$$

The stress state can be expressed in terms of the pressure and viscous component $\underline{\underline{\tau^{(i)}}}$ as:

$$\underline{\underline{\boldsymbol{T}^{(i)}}} = -P^{(i)} \, \underline{\underline{\boldsymbol{I}}} + \underline{\underline{\tau^{(i)}}} \tag{20}$$

Taking into account the conservation equations and Eqs. (4) and (7), the balance equations result:

$$\left(\mu^{(i)} + \kappa^{(i)} \right) \frac{\partial \rho^{(i)}}{\partial t} = -\nabla . \left[\rho^{(i)} \left(\mu^{(i)} + \kappa^{(i)} \right) \boldsymbol{V}^{(i)} \right] - C^{(i)} \left(\mu^{(i)} + \kappa^{(i)} \right) - \rho^{(i)} \, \boldsymbol{V}^{(i)} . \nabla \mu^{(i)} + \rho^{(i)} \, \boldsymbol{V}^{(i)} . \nabla \kappa^{(i)} \tag{21}$$

$$\boldsymbol{p}_v^{(i)} . \frac{\partial \boldsymbol{V}^{(i)}}{\partial t} = \nabla . \left(\underline{\underline{\tau^{(i)}}} . \boldsymbol{V}^{(i)} \right) - \rho^{(i)} \, \boldsymbol{V}^{(i)} . \nabla \kappa^{(i)} - \boldsymbol{V}^{(i)} . \nabla P^{(i)} + \boldsymbol{f}^{(i)} . \boldsymbol{V}^{(i)} - \underline{\underline{\tau^{(i)}}} : \nabla \boldsymbol{V}^{(i)} - 2 C^{(i)} \, \kappa^{(i)} + \rho^{(i)} \, \boldsymbol{G}^{(i)} . \boldsymbol{V}^{(i)} \tag{22}$$

$$\theta \frac{\partial s_v}{\partial t} = \sum_{i=1}^{r} \left\{ -\nabla . \left[\boldsymbol{q}^{(i)} + \left(\pi^{(i)} \, s_v - \mu^{(i)} \, \rho^{(i)} + \sum_{j=1}^{r} \mu^{(ij)} \, \rho^{(j)} \right) \boldsymbol{V}^{(i)} \right] + \boldsymbol{V}^{(i)} . \nabla P^{(i)} - \boldsymbol{f}^{(i)} . \boldsymbol{V}^{(i)} + \underline{\underline{\tau^{(i)}}} : \nabla \boldsymbol{V}^{(i)} + 2 C^{(i)} \, \kappa^{(i)} - C^{(i)} \left(\mu^{(i)} - \kappa^{(i)} \right) - \rho^{(i)} \, \boldsymbol{V}^{(i)} . \nabla \mu^{(i)} + \rho^{(i)} \, \Phi^{(i)} \right\} \tag{23}$$

According to the balance equations it can be seen that it is necessary to know, for each component, the potentials coming from the entropic representation of the internal energy and from the kinetic coenergy, as well as the mass and momentum interaction terms, the heat flux, the heat power source and the viscous stress.

The balance equations show one of the advantages of the BG-CFD methodology, that is, the representation of the power structure of the system. In the balance equations there can be identified three type of terms: divergence, source and coupling terms. The divergence terms take into account the power introduced in the system through the boundary conditions. The source terms constitute the different power sources, external to the system. Finally, the coupling terms represent power transfer between the velocity, mass and entropy equations; these coupling terms appear, with opposite signs, in pairs of balance equations. Taking into account Eq. (15) it verifies that coupling terms cancel out when the balance equations are added, resulting:

$$\frac{\partial e_v^*}{\partial t} = \sum_{i=1}^{r} \left\{ -\nabla . \left[\left(u_v^{(i)} + P^{(i)} - \rho^{(i)} \kappa^{(i)} \right) \boldsymbol{V}^{(i)} \right] + \nabla . \left(\underline{\underline{\tau^{(i)}}} . \boldsymbol{V}^{(i)} \right) - \nabla . \boldsymbol{q}^{(i)} + \rho^{(i)} \, \boldsymbol{G}^{(i)} . \boldsymbol{V}^{(i)} - \rho^{(i)} \, \Phi^{(i)} \right\} \tag{24}$$

The cancellation of the coupling terms means that they influence the power distribution among the different ports but not the total power in the system.

IV. DISCRETIZATION

The independent variables are discretized, in the domain volume Ω, in terms of time-dependent nodal values ($\rho_k^{(i)}$, $\boldsymbol{V}_m^{(i)}$ and s_{vl}) and interpolation (shape) functions correspondingly $\varphi_{\rho k}^{(i)}$, $\varphi_{Vm}^{(i)}$ and φ_{sl}):

$$\rho^{(i)}(\boldsymbol{r}, t) = \sum_{k=1}^{n_\rho^{(i)}} \rho_k^{(i)}(t) \, \varphi_{\rho k}^{(i)}(\boldsymbol{r}) = \underline{\rho^{(i)}}^T . \underline{\varphi_\rho^{(i)}} \tag{25}$$

$$\boldsymbol{V}^{(i)}(\boldsymbol{r}, t) = \sum_{m=1}^{n_V^{(i)}} \boldsymbol{V}_m^{(i)}(t) \, \varphi_{Vm}^{(i)}(\boldsymbol{r}) = \underline{\boldsymbol{V}^{(i)}}^T . \underline{\varphi_V^{(i)}} \tag{26}$$

$$s_v(\boldsymbol{r}, t) = \sum_{l=1}^{n_s} s_{vl}(t) \, \varphi_{sl}(\boldsymbol{r}) = \underline{s_v}^T . \underline{\varphi_s} \tag{27}$$

For any position $\boldsymbol{r} \in \Omega$, the shape functions have the following properties:

$$\sum_{k=1}^{n_\rho^{(i)}} \varphi_{\rho k}^{(i)}(\boldsymbol{r}) = 1 \;\; ; \;\; \sum_{m=1}^{n_V^{(i)}} \varphi_{Vm}^{(i)}(\boldsymbol{r}) = 1 \;\; ; \;\; \sum_{l=1}^{n_s} \varphi_{sl}(\boldsymbol{r}) = 1 \tag{28}$$

For simplicity in the treatment of the boundary conditions, we also require for the interpolation functions to have the value one for the reference node position, be monotonically decreasing with respect to the distance from the reference node and be zero for the rest of the nodes. Since this is the only discretization restriction, it is possible to work with any kind of grids. Notice that it is possible *a priori* to have different densification in the nodalization, this is, the number of nodes $n_\rho^{(i)}$ and $n_V^{(i)}$ can be different for each component; this is important, for instance, in boundary layer problems.

Nodal vectors are defined as Bond-Graph state variables, namely mass and velocity for the ith-component and entropy. The mass and entropy vectors are obtained by integrating the corresponding nodal independent variables in the support of the shape functions:

$$\underline{m^{(i)}} = \underline{\underline{\Omega_\rho^{(i)}}} \cdot \underline{\rho^{(i)}} \quad ; \quad \underline{S} = \underline{\underline{\Omega_s}} \cdot \underline{s_v} \tag{29}$$

The diagonal matrices $\underline{\underline{\Omega_\rho^{(i)}}}$ and $\underline{\underline{\Omega_s}}$ are defined as:

$$\underline{\underline{\Omega_\rho^{(i)}}} = \left\{\Omega_\rho^{(i)}\right\}_{kn} = \int_\Omega \varphi_{\rho k}^{(i)}\, \delta_{kn}\, d\Omega \tag{30}$$

$$\underline{\underline{\Omega_s}} = \{\Omega_s\}_{ln} = \int_\Omega \varphi_{sl}\, \delta_{ln}\, d\Omega \tag{31}$$

where δ_{ij} is the Kronecker's delta ($\delta_{ij} = 1$ if $i = j$, $\delta_{ij} = 0$ otherwise). The system mass for the ith-component and entropy are related to the integrated variables as follows:

$$m^{(i)} = \int_\Omega \rho^{(i)}\, d\Omega = \sum_{k=1}^{n_\rho^{(i)}} m_k^{(i)} \tag{32}$$

$$S = \int_\Omega s_v\, d\Omega = \sum_{l=1}^{n_s} S_l \tag{33}$$

The system total energy E^* is defined as the sum of the internal energy U and the kinetic coenergy T^*:

$$E^* = U(\underline{S}, \underline{m^{(1)}}, ..., \underline{m^{(r)}}) + T^*(\underline{m^{(1)}}, ..., \underline{m^{(r)}}, \underline{V^{(1)}}, ..., \underline{V^{(r)}}) \tag{34}$$

where:

$$E^* = \int_\Omega e_v^*\, d\Omega \quad ; \quad U = \int_\Omega u_v\, d\Omega \quad ; \quad T^* = \int_\Omega t_v^*\, d\Omega \tag{35}$$

From Eq. (35), it can be easily shown that the system kinetic coenergy can be expressed as the following bilinear form:

$$T^* = \sum_{i=1}^{r} \frac{1}{2}\, \underline{V^{(i)}}^T \cdot \underline{\underline{M^{(i)}}} \cdot \underline{V^{(i)}} \tag{36}$$

where $\underline{\underline{M^{(i)}}}$ is the inertia matrix corresponding to the ith-component:

$$\underline{\underline{M^{(i)}}} = \left\{M^{(i)}\right\}_{mn} = \int_\Omega \rho^{(i)}\, \varphi_{Vm}^{(i)}\, \varphi_{Vn}^{(i)}\, d\Omega \tag{37}$$

We define the following potentials:

$$\underline{\Theta} = \left(\frac{\partial U}{\partial \underline{S}}\right)_{\underline{m^{(i)}}} = \underline{\underline{\Omega_s}}^{-1} \cdot \left[\int_\Omega \theta\, \underline{\varphi_s}\, d\Omega\right] \tag{38}$$

$$\underline{\mu^{(i)}} = \left(\frac{\partial U}{\partial \underline{m^{(i)}}}\right)_{\underline{S}, \underline{m^{(j\neq i)}}} = \underline{\underline{\Omega_\rho^{(i)}}}^{-1} \cdot \left[\int_\Omega \mu^{(i)}\, \underline{\varphi_\rho^{(i)}}\, d\Omega\right] \tag{39}$$

$$\underline{K^{(i)}} = \left(\frac{\partial T^*}{\partial \underline{m^{(i)}}}\right)_{\underline{m^{(j\neq i)}}, \underline{V^{(k)}}} = \underline{\underline{\Omega_\rho^{(i)}}}^{-1} \cdot \left[\int_\Omega \kappa^{(i)}\, \underline{\varphi_\rho^{(i)}}\, d\Omega\right] \tag{40}$$

$$\underline{p^{(i)}} = \left(\frac{\partial T^*}{\partial \underline{V^{(i)}}}\right)_{\underline{m^{(j)}}, \underline{V^{(k\neq i)}}} = \underline{\underline{M^{(i)}}} \cdot \underline{V^{(i)}} = \int_\Omega \boldsymbol{p}_v^{(i)}\, \underline{\varphi_V^{(i)}}\, d\Omega \tag{41}$$

where $\underline{\Theta}$, $\underline{\mu^{(i)}}$, $\underline{K^{(i)}}$ and $\underline{p^{(i)}}$ are correspondingly nodal vectors of temperature and chemical potential per unit mass, kinetic coenergy per unit mass and linear momentum for the ith-component. It is important to notice that Eq. (41) defines, in the Bond-Graph terminology, a modulated multibond transformer relating the nodal vectors of velocity and linear momentum for the ith-component, as shown in Fig. 1; in this and in the following figures, it is drawn the causality resulting from the Bond-Graph causality assignment procedure [7]. According to

Fig. 1. Modulated ith-component inertial transformer.

the power conservation across the transformer, the generalized effort is given by:

$$\underline{F^{(i)}} = \underline{\underline{M^{(i)}}} \cdot \underline{\dot{V}^{(i)}} \tag{42}$$

According to Eq. (41), the nodal vector of ith-component linear momentum can be regarded as a system volume integral of the local values weighted by the velocity interpolation function. It can be easily shown that the system ith-component linear momentum can be obtained as:

$$\boldsymbol{p}^{(i)} = \int_\Omega \boldsymbol{p}_v^{(i)}\, d\Omega = \sum_{m=1}^{n_V^{(i)}} \boldsymbol{p}_m^{(i)} \tag{43}$$

According to Eqs. (38) to (40), the nodal vectors $\underline{\Theta}$, $\underline{\mu^{(i)}}$ and $\underline{K^{(i)}}$ can be regarded as system volume averages of the corresponding local values, weighted by the interpolation functions. The time derivative of the system total energy can be written as:

$$\dot{E}^* = \underline{\Theta}^T \cdot \underline{\dot{S}} + \sum_{i=1}^{r} \left[\left(\underline{\mu^{(i)}} + \underline{K^{(i)}}\right)^T \cdot \underline{\dot{m}^{(i)}} - \underline{p^{(i)}}^T \cdot \underline{\dot{V}^{(i)}}\right] \tag{44}$$

It can also be shown that the volume integrals of the left side terms of Eqs. (21) to (23) can be calculated as:

$$\int_\Omega \left(\mu^{(i)} + \kappa^{(i)}\right) \frac{\partial \rho^{(i)}}{\partial t}\, d\Omega = \left(\underline{\mu^{(i)}} + \underline{K^{(i)}}\right)^T \cdot \underline{\dot{m}^{(i)}} \tag{45}$$

$$\int_\Omega \boldsymbol{p}_v^{(i)} \cdot \frac{\partial \boldsymbol{V}^{(i)}}{\partial t}\, d\Omega = \underline{p^{(i)}}^T \cdot \underline{\dot{V}^{(i)}} \tag{46}$$

$$\int_\Omega \theta\, \frac{\partial s_v}{\partial t}\, d\Omega = \underline{\Theta}^T \cdot \underline{\dot{S}} \tag{47}$$

The Maxwell relations corresponding to the system total energy arise from the equality of the mixed partial derivatives of the system total energy expressed as a function of the independent variables $\underline{S}$, $\underline{m^{(i)}}$ and $\underline{V^{(i)}}$. These variables are regarded as the state variables for the BG-CFD methodology:

$$\left(\frac{\partial \underline{\Theta}}{\partial \underline{m^{(i)}}}\right)_{\underline{S}, \underline{m^{(j\neq i)}}} = \left(\frac{\partial \underline{\mu^{(i)}}}{\partial \underline{S}}\right)^T_{\underline{m^{(j)}}} \tag{48}$$

$$\left(\frac{\partial \underline{\Theta}}{\partial \underline{V^{(i)}}}\right)_{\underline{S}, \underline{m^{(j)}}} = \left(\frac{\partial \underline{p^{(i)}}}{\partial \underline{S}}\right)^T_{\underline{m^{(i)}}, \underline{V^{(i)}}} = \underline{\underline{0}} \tag{49}$$

$$\left(\frac{\partial \underline{p^{(i)}}}{\partial \underline{m^{(j)}}}\right)_{\underline{V^{(i)}}} = \left(\frac{\partial \underline{K^{(j)}}}{\partial \underline{V^{(i)}}}\right)^T \tag{50}$$

The constitutive relations, Eqs. (38) to (41), and the Maxwell relations, Eqs. (48) to (50) define, in the Bond-Graph terminology, a multibond IC-field associated to the system total energy, as shown in Fig. 2. This field has r inertial ports (the velocity ports) and $r - 1$ capacitive ports (the entropy port and the r mass ports). The generalized effort variables associated to these ports are $\underline{\dot{V}^{(i)}}$, $\underline{\Theta}$ and $\left(\underline{\mu^{(i)}} + \underline{K^{(i)}}\right)$, while the generalized flow variables are correspondingly $\underline{p^{(i)}}$, $\underline{\dot{S}}$ and $\underline{\dot{m}^{(i)}}$.

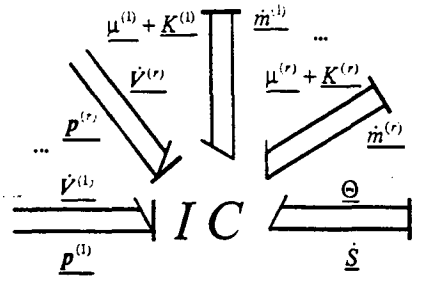

Fig. 2. System *IC*-field representing energy storage.

For the sake of convenience, we also define the following diagonal matrices, whose elements are the components of the corresponding vectors of nodal potentials:

$$\underline{\underline{\Theta}} = \{\Theta\}_{ln} = \Theta_l\,\delta_{ln} \tag{51}$$

$$\underline{\underline{\mu^{(i)}}} = \left\{\mu^{(i)}\right\}_{kn} = \mu_k^{(i)}\,\delta_{kn} \tag{52}$$

$$\underline{\underline{K^{(i)}}} = \left\{K^{(i)}\right\}_{kn} = K_k^{(i)}\,\delta_{kn} \tag{53}$$

V. SYSTEM STATE EQUATIONS

The system state equations are obtained by systematically volume integrating the balance equations corresponding to each port of the *IC*-field representing the total system energy. The expressions for the system state equations are:

$$\underline{\dot{m}^{(i)}} = \underline{\dot{m}_W^{(\Gamma)(i)}} + \underline{\dot{m}_{WF}^{(i)}} + \underline{\dot{m}_U^{(i)}} + \underline{\dot{m}_{CK}^{(i)}} + \underline{\dot{m}_K^{(i)}} \tag{54}$$

$$\underline{\dot{V}^{(i)}} = \underline{\underline{M^{(i)}}}^{-1}.\left(\underline{\boldsymbol{F}_T^{(\Gamma)(i)}} - \underline{\boldsymbol{F}_K^{(i)}} - \underline{\boldsymbol{F}_P^{(i)}} - \underline{\boldsymbol{F}_D^{(i)}} - \underline{\boldsymbol{F}_C^{(i)}} - \underline{\boldsymbol{F}_G^{(i)}}\right) \tag{55}$$

$$\underline{\dot{S}} = \underline{\dot{S}_Q^{(\Gamma)}} + \underline{\dot{S}_{QF}} - \underline{\dot{S}_P} + \underline{\dot{S}_D} + \underline{\dot{S}_C} - \underline{\dot{S}_U} - \underline{\dot{S}_{CK}} + \underline{\dot{S}_F} \tag{56}$$

The different terms in the system state equations (54) to (56) arise from integrations over the domain volume Ω or the domain boundary Γ. Their definitions are:

$$\underline{\dot{m}_W^{(\Gamma)(i)}} = -\underline{\underline{E_M^{(i)}}}.\left[\int_\Gamma \underline{w_\rho^{(i)}}\,\rho^{(i)}\left(\mu^{(i)} - \kappa^{(i)}\right) V^{(i)}.\check{\mathbf{n}}\,d\Gamma\right] \tag{57}$$

$$\underline{\dot{m}_{WF}^{(i)}} = \underline{\underline{E_M^{(i)}}}.\left[\int_\Omega \rho^{(i)}\left(\mu^{(i)} - \kappa^{(i)}\right) V^{(i)}.\nabla\underline{w_\rho^{(i)}}\,d\Omega\right] \tag{58}$$

$$\underline{\dot{m}_U^{(i)}} = \underline{\underline{E_M^{(i)}}}.\left[\int_\Omega \underline{w_\rho^{(i)}}\,\rho^{(i)}\,V^{(i)}.\nabla\mu^{(i)}\,d\Omega\right] \tag{59}$$

$$\underline{\dot{m}_{CK}^{(i)}} = \underline{\underline{E_M^{(i)}}}.\left[\int_\Omega \underline{w_\rho^{(i)}}\,C^{(i)}\left(\mu^{(i)} + \kappa^{(i)}\right) d\Omega\right] \tag{60}$$

$$\underline{\dot{m}_K^{(i)}} = \underline{\underline{E_M^{(i)}}}.\left[\int_\Omega \underline{w_\rho^{(i)}}\,\rho^{(i)}\,V^{(i)}.\nabla\kappa^{(i)}\,d\Omega\right] \tag{61}$$

$$\underline{\boldsymbol{F}_T^{(\Gamma)(i)}} = \int_\Gamma \left(\underline{\underline{\tau^{(i)}}}.\check{\mathbf{n}}\right)\underline{\varphi_V^{(i)}}\,d\Gamma \tag{62}$$

$$\underline{\boldsymbol{F}_K^{(i)}} = \int_\Omega \rho^{(i)}\,\nabla\kappa^{(i)}\,\underline{\varphi_V^{(i)}}\,d\Omega \tag{63}$$

$$\underline{\boldsymbol{F}_P^{(i)}} = \int_\Omega \left(\nabla P^{(i)} - \boldsymbol{f}^{(i)}\right)\underline{\varphi_V^{(i)}}\,d\Omega \tag{64}$$

$$\underline{\boldsymbol{F}_D^{(i)}} = \int_\Omega \underline{\underline{\tau^{(i)}}}.\nabla\underline{\varphi_V^{(i)}}\,d\Omega \tag{65}$$

$$\underline{\boldsymbol{F}_C^{(i)}} = -\int_\Omega C^{(i)}\,V^{(i)}\,\underline{\varphi_V^{(i)}}\,d\Omega \tag{66}$$

$$\underline{\boldsymbol{F}_G^{(i)}} = \int_\Omega \rho^{(i)}\,G^{(i)}\,\underline{\varphi_V^{(i)}}\,d\Omega \tag{67}$$

$$\underline{\dot{S}_Q^{(\Gamma)}} = \underline{\underline{\Theta}}^{-1}.\left\{-\int_\Gamma \underline{w_s}\sum_{i=1}^{r}\left[q^{(i)} + \left(\pi^{(i)}\,s_v - \mu^{(i)}\,\rho^{(i)} + \sum_{j=1}^{r}\mu^{(ij)}\,\rho^{(j)}\right)V^{(i)}\right].\check{\mathbf{n}}\,d\Gamma\right\} \tag{68}$$

$$\underline{\dot{S}_{QF}} = \underline{\underline{\Theta}}^{-1}.\left\{\int_\Omega \nabla\underline{w_s}.\sum_{i=1}^{r}\left[q^{(i)} + \left(\pi^{(i)}\,s_v - \mu^{(i)}\,\rho^{(i)} + \sum_{j=1}^{r}\mu^{(ij)}\,\rho^{(j)}\right)V^{(i)}\right]d\Omega\right\} \tag{69}$$

$$\underline{\dot{S}_F} = \underline{\underline{\Theta}}^{-1}.\left[\int_\Omega \underline{w_s}\left(\sum_{i=1}^{r}\rho^{(i)}\,\Phi^{(i)}\right)d\Omega\right] \tag{70}$$

$$\underline{\dot{S}_P} = \sum_{i=1}^{r}\underline{\dot{S}_P^{(i)}}\;;\;\underline{\dot{S}_D} = \sum_{i=1}^{r}\underline{\dot{S}_D^{(i)}}\;;\;\underline{\dot{S}_C} = \sum_{i=1}^{r}\underline{\dot{S}_C^{(i)}} \tag{71}$$

$$\underline{\dot{S}_U} = \sum_{i=1}^{r}\underline{\dot{S}_U^{(i)}}\;;\;\underline{\dot{S}_{CK}} = \sum_{i=1}^{r}\underline{\dot{S}_{CK}^{(i)}} \tag{72}$$

where:

$$\underline{\underline{E_M^{(i)}}} = \left(\underline{\underline{\mu^{(i)}}} + \underline{\underline{K^{(i)}}}\right)^{-1} \tag{73}$$

$$\underline{\dot{S}_P^{(i)}} = \underline{\underline{\Theta}}^{-1}.\left[\int_\Omega \underline{w_s}\left(\nabla P^{(i)} - \boldsymbol{f}^{(i)}\right).V^{(i)}d\Omega\right] \tag{74}$$

$$\underline{\dot{S}_D^{(i)}} = \underline{\underline{\Theta}}^{-1}.\left[\int_\Omega \underline{w_s}\left(\nabla V^{(i)} : \underline{\underline{\tau^{(i)}}}\right)d\Omega\right] \tag{75}$$

$$\underline{\dot{S}_C^{(i)}} = \underline{\underline{\Theta}}^{-1}.\left[-\int_\Omega \underline{w_s}\,2\,C^{(i)}\,\kappa^{(i)}d\Omega\right] \tag{76}$$

$$\underline{\dot{S}_U^{(i)}} = \underline{\underline{\Theta}}^{-1}.\left[\int_\Omega \underline{w_s}\,\rho^{(i)}\,V^{(i)}.\nabla\mu^{(i)}\,d\Omega\right] \tag{77}$$

$$\underline{\dot{S}_{CK}^{(i)}} = \underline{\underline{\Theta}}^{-1}.\left[\int_\Omega \underline{w_s}\,C^{(i)}\left(\mu^{(i)} + \kappa^{(i)}\right)d\Omega\right] \tag{78}$$

Although the complete Bond Graph is not shown here, it can be said that the state equations (54) and (56) are represented, in the Bond-Graph terminology, by multibond 0-junctions, in which correspondingly the ith-component mass rate nodal vectors and the entropy rate nodal vector are added (see Figs. 3 and 4). Eq. (55) is represented, in the Bond-Graph terminology, by a multibond 1-junction, in which the forces are added (see Fig. 5). A multibond 0-junction is also used to represent Eqs. (71) and (72).

The convective (upwind) nature of the fluid equations is handled through the definition of density and entropy weight functions, namely $\underline{w_\rho^{(i)}}$ and $\underline{w_s}$, which are introduced to satisfy the power interchanged by the system through the boundary conditions, as well as to share the importance of different power

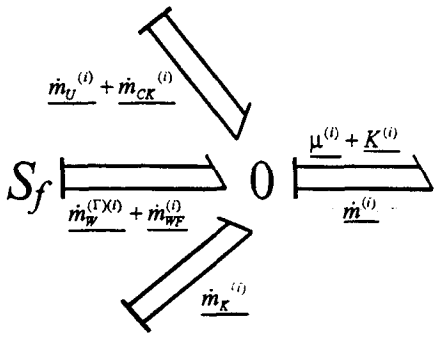

Fig. 3. 0-junction representing the balance equation at the ith-component mass port.

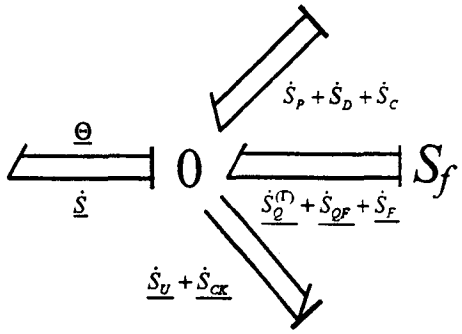

Fig. 4. 0-junction representing the balance equation at the entropy port.

terms among neighboring nodes. In the discretization procedure, all the terms of the ith-component mass balance equation and entropy balance equation were multiplied correspondingly by $w_\rho^{(i)}$ and w_s; although this procedure has the advantage that the steady-state balance equations are satisfied locally for the different nodes, other discretization strategies are possible and should be investigated. This concept was successfully applied to convection-diffusion problems [8][9]. It is very interesting to notice that, according to this Bond-Graph methodology, no weight functions result for the velocity state equations.

As in [1], all kind of boundary conditions can be handled consistently through the terms representing surface integrals ($\dot{m}_W^{(\Gamma)(i)}$, $\underline{F}_T^{(\Gamma)(i)}$ and $\dot{S}_Q^{(\Gamma)}$) and can be represented (in the Bond-Graph terminology) either as generalized modulated effort sources at the inertial ports or modulated flow sources at

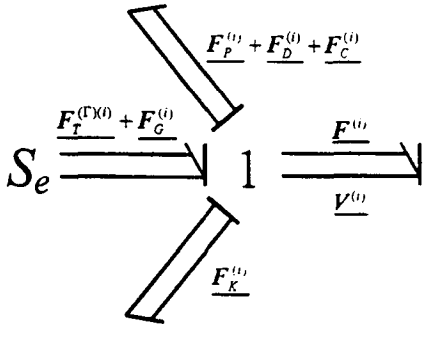

Fig. 5. 1-junction representing the balance equation at the ith-component velocity port.

the capacitive ports, as shown in Figs. 3 to 5.

The discretized representation of the power coupling appearing in the balance equations per unit volume is performed through the coupling matrices, which relate generalized variables whose product gives rise to power terms appearing in more than one port. Depending on the variables being related, these matrices define, in the Bond-Graph terminology, power conserving two-port elements (modulated transformers or modulated gyrators), as shown in Figs. 6 to 8.

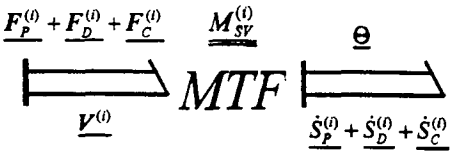

Fig. 6. Power coupling between the ith-component velocity and entropy ports.

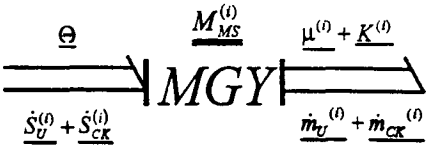

Fig. 7. Power coupling between the ith-component entropy and mass ports.

Fig. 8. Power coupling between the ith-component velocity and mass ports.

It can be shown that the relationships corresponding to Figs. 6 to 8 are:

$$\underline{F}_P^{(i)} + \underline{F}_D^{(i)} - \underline{F}_C^{(i)} = \underline{\underline{M}}_{SV}^{(i)} \cdot \Theta \tag{79}$$

$$\dot{S}_P^{(i)} - \dot{S}_D^{(i)} - \dot{S}_C^{(i)} = \underline{\underline{M}}_{SV}^{(i)\,T} \cdot V^{(i)} \tag{80}$$

$$\dot{S}_U^{(i)} - \dot{S}_{CK}^{(i)} = \underline{\underline{M}}_{MS}^{(i)} \cdot \left(\mu^{(i)} - K^{(i)}\right) \tag{81}$$

$$\dot{m}_U^{(i)} + \dot{m}_{CK}^{(i)} = \underline{\underline{M}}_{MS}^{(i)\,T} \cdot \Theta \tag{82}$$

$$\underline{F}_K^{(i)} = \underline{\underline{M}}_{MV}^{(i)} \cdot \left(\mu^{(i)} - K^{(i)}\right) \tag{83}$$

$$\dot{m}_K^{(i)} = \underline{\underline{M}}_{MV}^{(i)\,T} \cdot \underline{V}^{(i)} \tag{84}$$

where the rectangular matrices $\underline{\underline{M}}_{SV}^{(i)}$ ($n_V^{(i)}$ rows, n_s columns), $\underline{\underline{M}}_{MS}^{(i)}$ (n_s rows, $n_\rho^{(i)}$ columns) and $\underline{\underline{M}}_{MV}^{(i)}$ ($n_V^{(i)}$ rows, $n_\rho^{(i)}$ columns) are defined as:

$$\left\{\underline{\underline{M}}_{SV}^{(i)}\right\}_{ml} = \frac{1}{\Theta_l} \int_\Omega \left[\left(\nabla P^{(i)} - f^{(i)} - C^{(i)}\,V^{(i)}\right) \varphi_{Vm}^{(i)} + \underline{\underline{T}}^{(i)} \cdot \nabla \varphi_{Vm}^{(i)}\right] w_{sl}\, d\Omega \tag{85}$$

$$\left\{\underline{\underline{M}}^{(i)}_{MS}\right\}_{lk} = \frac{1}{\Theta_l}\frac{1}{\mu^{(i)}_k + K^{(i)}_k}\int_\Omega \rho^{(i)}\, V^{(i)}.\nabla\mu^{(i)} + C^{(i)}\left(\mu^{(i)} + \kappa^{(i)}\right)\Big] w_{sl}\, w^{(i)}_{pk}\, d\Omega \quad (86)$$

$$\left\{\underline{\underline{M}}^{(i)}_{MV}\right\}_{mk} = \frac{1}{\mu^{(i)}_k + K^{(i)}_k}\int_\Omega \rho^{(i)}\,\nabla\kappa^{(i)}\,\varphi^{(i)}_{Vm}\, d\Omega \quad (87)$$

Since the coupling matrices relate nodal vectors which may have different sizes, they are rectangular and may be not inversible, setting a restriction in the allowable causalities. For instance, from Fig. 8 and Eqs. (79) and (80) it can be seen that the input variables to the ports of the modulated transformer must be $\underline{\Theta}$ and $\mathbf{V}^{(i)}$, while the output variables result correspondingly the nodal forces and the nodal entropy rates for the ith-component.

Finally, initial conditions are needed for the nodal vectors of state variables. If initial conditions are given as continuous functions, these nodal vectors are determined in such a way that the ith-component total mass and momentum, as well as the total entropy, is kept constant after the discretization.

VI. MIXTURE OF IDEAL GASES

As an application example, the potentials defined in Section are calculated for a multicomponent solution (mixture) of ideal gases. The entropic representation of the internal energy for an ideal gas is [5]:

$$u^{(i)}_v = \frac{\rho^{(i)}}{\rho^{(i)}_0}u^{(i)}_{v0} + \frac{\rho^{(i)}}{M^{(i)}}\int_{\theta_0}^{\theta} c^{(i)}_v(\theta')\, d\theta' \quad (88)$$

$$s_v = \sum_{i=1}^{r}\left[\frac{\rho^{(i)}}{\rho^{(i)}_0}s^{(i)}_{v0} + \frac{\rho^{(i)}}{M^{(i)}}\int_{\theta_0}^{\theta}\frac{c^{(i)}_v(\theta')}{\theta'}d\theta' - \frac{\rho^{(i)}}{M^{(i)}}R\ln\left(\frac{\rho^{(i)}_0}{\rho^{(i)}}\right)\right] \quad (89)$$

where R is a universal constant, θ_0 are the temperature at a reference state, $\rho^{(i)}_0$, $u^{(i)}_{v0}$ and $s^{(i)}_{v0}$ are correspondingly the density, internal energy per unit volume and entropy per unit volume for the ith-component at the reference state, $M^{(i)}$ is the ith-component molar mass and $c^{(i)}_v$ is the ith-component specific heat at constant volume (function of temperature only). Eqs. (88) and (89) are a representation of Eq. (5) in parametric form, being the parameter the temperature θ. From this representation, the potentials result:

$$\pi^{(i)} = \theta\frac{\frac{\rho^{(i)}}{M^{(i)}}c^{(i)}_v}{\left(\sum_{j=1}^{r}\frac{\rho^{(j)}}{M^{(j)}}c^{(j)}_v\right)} \quad (90)$$

$$\mu^{(ij)} = \left(\frac{u^{(i)}_{v0}}{\rho^{(i)}_0} + \frac{1}{M^{(i)}}\int_{\theta_0}^{\theta}c^{(i)}_v(\theta')\,d\theta'\right)\delta_{ij} - \pi^{(i)}\left[\frac{s^{(j)}_{v0}}{\rho^{(j)}_0} - \frac{1}{M^{(j)}}\int_{\theta_0}^{\theta}\frac{c^{(j)}_v(\theta')}{\theta'}d\theta' + \frac{R}{M^{(j)}}\ln\left(\frac{\rho^{(j)}}{\rho^{(j)}_0}\right) - \frac{R}{M^{(j)}}\right] \quad (91)$$

$$P^{(i)} = P\frac{\frac{\rho^{(i)}}{M^{(i)}}c^{(i)}_v}{\left(\sum_{j=1}^{r}\frac{\rho^{(j)}}{M^{(j)}}c^{(j)}_v\right)} \quad (92)$$

where the total pressure results:

$$P = \left(\sum_{i=1}^{r}\frac{\rho^{(i)}}{M^{(i)}}\right)R\theta$$

From Eqs. (90) and (92), it can be seen that the contributions to the total temperature and pressure from the ith-component are weighted by the product of the molar density and the specific heat.

VII. CONCLUSIONS

In this paper, the BG-CFD methodology was extended to Multicomponent Solutions. The multivelocity model were presented, leaving the presentation of the diffusion model for a separate contribution [6].

Based on the total energy per unit volume, the BG-CFD methodology allowed to define a set of independent variables, potentials and constitutive relations needed to describe a multicomponent system.

The state equations were obtained by systematically integrating a set of power balance equations. These balance equations, obtained from Continuum Theory, take into account all physical effects (convection, heat transfer, compressibility, inertia, reaction, etc.) encountered in multicomponent solutions. The resulting Bond Graph represents the power structure of the system, showing energy storage, power interchange through the boundary conditions, power sources and power couplings between the different ports.

The author believes that the BG-CFD methodology is the foundation of a bridge between Bond Graphs and Computational Fluid Dynamics. It is hoped that the findings of this paper encourage other researchers to use this formalism in more specific problems.

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