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A New Approach for Modeling Multicomponent Solutions

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Abstract— This paper shows an application to Multicomponent Solutions of a new, Bond-Graph based formalism for Computational Fluid Dynamics (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. Based on the multiveLOCITY model, the diffusion approximation is presented. This model differs from the multiveLOCITY model in the way the kinetic coenergy of the components is taken into account, reducing the number of state variables from multiple velocities to a mean velocity. In the diffusion model, 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. The relative fluxes are assumed to be dependent on the entropy per unit volume and the component densities. This functional dependence allows to deal with ordinary (concentration driven) diffusion, pressure diffusion, forced diffusion and thermal diffusion. Based on the contribution of the diffusion fluxes to the kinetic coenergy, different potentials associated to the entropy per unit volume and component densities are defined. It is shown that these potentials modify the generalized effort variables appearing at the inertial, mass and thermal ports of the IC-field representing the system total energy. Besides, these potentials introduce linkages between these ports.

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

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 [4] 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 [5] 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 used in this paper, bold

letters will be used to define first order tensors ($V^{(i)}$, $p_v^{(i)}$, etc.). Column vectors associated to nodal values will be denoted by single underscored plain or bold type ($\underline{m}^{(i)}$, $\underline{g}^{(i)}$, $\underline{V}^{(i)}$, $\underline{\varphi}_\rho^{(i)}$, etc.) while multidimensional matrices will be identified by double underscored plain type ($\underline{\underline{M}}^{(i)}$, $\underline{\underline{\Omega}}_\rho^{(i)}$, etc.). Second order tensors will be denoted by bold, double underscored type ($\underline{\underline{\tau}}^{(i)}$, $\underline{\underline{I}}$, etc.). 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 $\rho^{(i)}$:

$$u_v = u_v(s_v, \rho^{(1)}, \dots, \rho^{(r)}) \quad (1)$$

The following potentials are defined:

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

where θ is the temperature and $\mu^{(i)}$ is the i th-component chemical potential per unit mass. The pressure P can be obtained from the Euler equation [6]:

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

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

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

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

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

The following potentials are defined:

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

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

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

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

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

the following relations are verified:

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

As an example, the potentials associated to the entropic representation of the i th-component internal energy are calculated in Section VII 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 $V^{(i)}$:

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

The following potentials are defined:

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

$$p_v^{(i)} = \left(\frac{\partial t_v^*}{\partial V^{(i)}} \right)_{\rho^{(j)}, V^{(k \neq i)}} = \rho^{(i)} V^{(i)} \quad (12)$$

where $\kappa^{(i)}$ and $p_v^{(i)}$ are correspondingly the kinetic coenergy per unit mass and linear momentum per unit mass for the i th-component. The time derivative of the kinetic coenergy per unit volume can be written as:

$$\frac{\partial t_v^*}{\partial t} = \sum_{i=1}^r \kappa^{(i)} \frac{\partial \rho^{(i)}}{\partial t} + \sum_{i=1}^r p_v^{(i)} \cdot \frac{\partial V^{(i)}}{\partial t} \quad (13)$$

C. Total Energy per Unit Volume

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

$$e_v^* = u_v + t_v^* \quad (14)$$

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

$$\frac{\partial e_v^*}{\partial t} = \theta \frac{\partial s_v}{\partial t} + \sum_{i=1}^r \left[(\mu^{(i)} + \kappa^{(i)}) \frac{\partial \rho^{(i)}}{\partial t} + p_v^{(i)} \cdot \frac{\partial V^{(i)}}{\partial t} \right] \quad (15)$$

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 from Thermodynamics [6].

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 multi-component solutions, the balance equations can be derived from the mass, momentum and energy conservation equation corresponding to each component [5]:

$$\frac{\partial \rho^{(i)}}{\partial t} = -\nabla \cdot (\rho^{(i)} V^{(i)}) + C^{(i)} \quad (16)$$

$$\rho^{(i)} \frac{\partial V^{(i)}}{\partial t} = -\rho^{(i)} V^{(i)} \cdot \nabla V^{(i)} + \nabla \cdot \underline{\underline{T}}^{(i)} + \rho^{(i)} G^{(i)} + f^{(i)} - C^{(i)} V^{(i)} \quad (17)$$

$$\frac{\partial u_v^{(i)}}{\partial t} = -\nabla \cdot (u_v^{(i)} V^{(i)}) - f^{(i)} \cdot V^{(i)} + C^{(i)} \frac{1}{2} V^{(i)2} + \underline{\underline{T}}^{(i)} : \nabla V^{(i)} + \rho^{(i)} \Phi^{(i)} - \nabla \cdot q^{(i)} + \epsilon^{(i)} \quad (18)$$

where $C^{(i)}$, $f^{(i)}$ 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, $G^{(i)}$ is the body force, $q^{(i)}$ is the heat flux and $\underline{\underline{T}}^{(i)}$ is the stress state for the i th-component.

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

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

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

$$\underline{\underline{T}}^{(i)} = -P^{(i)} \underline{\underline{I}} + \underline{\underline{T}}^{(i)} \quad (20)$$

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

$$\begin{aligned} (\mu^{(i)} + \kappa^{(i)}) \frac{\partial \rho^{(i)}}{\partial t} = & -\nabla \cdot [\rho^{(i)} (\mu^{(i)} + \kappa^{(i)}) V^{(i)}] \\ & + C^{(i)} (\mu^{(i)} + \kappa^{(i)}) + \rho^{(i)} V^{(i)} \cdot \nabla \mu^{(i)} + \rho^{(i)} V^{(i)} \cdot \nabla \kappa^{(i)} \end{aligned} \quad (21)$$

$$\begin{aligned} p_v^{(i)} \cdot \frac{\partial V^{(i)}}{\partial t} = & \nabla \cdot (\underline{\underline{T}}^{(i)} \cdot V^{(i)}) - \rho^{(i)} V^{(i)} \cdot \nabla \kappa^{(i)} - V^{(i)} \cdot \nabla P^{(i)} \\ & + f^{(i)} \cdot V^{(i)} - \underline{\underline{T}}^{(i)} : \nabla V^{(i)} - 2 C^{(i)} \kappa^{(i)} + \rho^{(i)} G^{(i)} \cdot V^{(i)} \end{aligned} \quad (22)$$

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

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 balance equations; these coupling terms appear, with opposite signs, in pairs of equations. Taking into account Eq. (15) it verifies that coupling terms cancel out when the balance equations are added, resulting:

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

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 ($\rho_k^{(i)}$, $\mathbf{V}_m^{(i)}$ and s_{vl}) and interpolation (shape) functions (correspondingly $\varphi_{\rho k}^{(i)}$, $\varphi_{V_m}^{(i)}$ and φ_{sl}):

$$\rho^{(i)}(\mathbf{r}, t) = \sum_{k=1}^{n_\rho^{(i)}} \rho_k^{(i)}(t) \varphi_{\rho k}^{(i)}(\mathbf{r}) = \underline{\underline{\rho}}^{(i)T} \cdot \underline{\underline{\varphi}}_\rho^{(i)} \quad (25)$$

$$\mathbf{V}^{(i)}(\mathbf{r}, t) = \sum_{m=1}^{n_V^{(i)}} \mathbf{V}_m^{(i)}(t) \varphi_{V_m}^{(i)}(\mathbf{r}) = \underline{\underline{\mathbf{V}}}^{(i)T} \cdot \underline{\underline{\varphi}}_V^{(i)} \quad (26)$$

$$s_v(\mathbf{r}, t) = \sum_{l=1}^{n_s} s_{vl}(t) \varphi_{sl}(\mathbf{r}) = \underline{\underline{s}}_v^T \cdot \underline{\underline{\varphi}}_s \quad (27)$$

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

$$\sum_{k=1}^{n_\rho^{(i)}} \varphi_{\rho k}^{(i)}(\mathbf{r}) = 1 ; \quad \sum_{m=1}^{n_V^{(i)}} \varphi_{V_m}^{(i)}(\mathbf{r}) = 1 ; \quad \sum_{l=1}^{n_s} \varphi_{sl}(\mathbf{r}) = 1 \quad (28)$$

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 i th-component and entropy. The mass and entropy vectors are obtained by integrating the corresponding nodal independent variables in the support of the shape functions:

$$\underline{\underline{m}}^{(i)} = \underline{\underline{\Omega}}_\rho^{(i)} \cdot \underline{\underline{\rho}}^{(i)} ; \quad \underline{\underline{S}} = \underline{\underline{\Omega}}_s \cdot \underline{\underline{s}}_v \quad (29)$$

The diagonal matrices $\underline{\underline{\Omega}}_\rho^{(i)}$ and $\underline{\underline{\Omega}}_s$ are defined as:

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

$$\underline{\underline{\Omega}}_s = \{ \Omega_{sl} \} = \int_\Omega \varphi_{sl} \delta_{ln} d\Omega \quad (31)$$

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

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

$$S = \int_\Omega s_v d\Omega = \sum_{l=1}^{n_s} S_l \quad (33)$$

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

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

where:

$$E^* = \int_\Omega e_v^* d\Omega ; \quad U = \int_\Omega u_v d\Omega ; \quad T^* = \int_\Omega t_v^* d\Omega \quad (35)$$

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



Fig. 1. Modulated ith-component inertial transformer.

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

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

$$\underline{M}^{(i)} = \{M_{mn}^{(i)}\} = \int_{\Omega} \rho^{(i)} \varphi_{V_m}^{(i)} \varphi_{V_n}^{(i)} d\Omega \quad (37)$$

We define the following potentials:

$$\underline{\Theta} = \left(\frac{\partial U}{\partial \underline{\mathcal{S}}} \right)_{\underline{m}^{(j)}} = \underline{\Omega}_g^{-1} \cdot \left[\int_{\Omega} \theta \varphi_g d\Omega \right] \quad (38)$$

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

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

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

where $\underline{\Theta}$, $\underline{\mu}^{(i)}$, $\underline{K}^{(i)}$ and $\underline{p}^{(i)}$ are correspondingly nodal vectors of temperature and ith-component chemical potential per unit mass, kinetic coenergy per unit mass and linear momentum. 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, 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 [4]. According to the power conservation across the transformer, the generalized effort is given by:

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

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:

$$\underline{p}^{(i)} = \int_{\Omega} p_v^{(i)} d\Omega = \sum_{m=1}^{n_v^{(i)}} p_m^{(i)} \quad (43)$$

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:

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

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

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

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

$$\int_{\Omega} \theta \frac{\partial s_v}{\partial t} d\Omega = \underline{\Theta}^T \cdot \dot{\underline{\mathcal{S}}} \quad (47)$$

The system constitutive relations are:

$$\underline{\mu}^{(i)} + \underline{K}^{(i)} = \underline{\mu}^{(i)} \left(\underline{\mathcal{S}}, \underline{m}^{(1)}, \dots, \underline{m}^{(r)} \right) + \underline{K}^{(i)} \left(\underline{V}^{(i)} \right) \quad (48)$$

$$\underline{p}^{(i)} = \underline{p}^{(i)} \left(\underline{m}^{(i)}, \underline{V}^{(i)} \right) = \underline{M}^{(i)} \cdot \underline{V}^{(i)} \quad (49)$$

$$\underline{\Theta} = \underline{\Theta} \left(\underline{\mathcal{S}}, \underline{m}^{(1)}, \dots, \underline{m}^{(r)} \right) \quad (50)$$

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 $\underline{\mathcal{S}}$, $\underline{m}^{(i)}$ and $\underline{V}^{(i)}$. These variables are regarded as the state variables for the BG-CFD methodology:

$$\left(\frac{\partial \underline{\Theta}}{\partial \underline{m}^{(i)}} \right)_{\underline{\mathcal{S}}, \underline{m}^{(j \neq i)}} = \left(\frac{\partial \underline{\mu}^{(i)}}{\partial \underline{\mathcal{S}}} \right)_{\underline{m}^{(j)}}^T \quad (51)$$

$$\left(\frac{\partial \underline{\Theta}}{\partial \underline{V}^{(i)}} \right)_{\underline{\mathcal{S}}, \underline{m}^{(j)}} = \left(\frac{\partial \underline{p}^{(i)}}{\partial \underline{\mathcal{S}}} \right)_{\underline{m}^{(i)}, \underline{V}^{(i)}}^T = \underline{0} \quad (52)$$

$$\left(\frac{\partial \underline{p}^{(i)}}{\partial \underline{m}^{(j)}} \right)_{\underline{V}^{(i)}} = \left(\frac{\partial \underline{K}^{(j)}}{\partial \underline{V}^{(i)}} \right)^T \quad (53)$$

The constitutive relations (Eqs. (48) to (50)) and the Maxwell relations (Eqs. (51) to (53)) 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 $\underline{p}^{(i)}$, $\dot{\underline{\mathcal{S}}}$ and $\dot{\underline{m}}^{(i)}$.

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

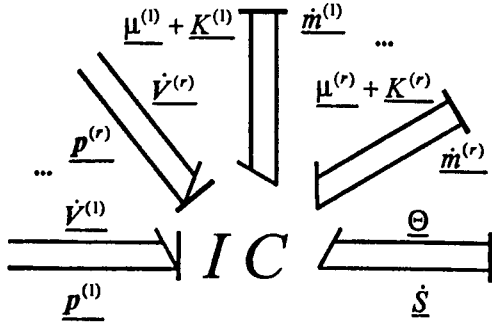


Fig. 2. System IC field representing energy storage.

$$\underline{\Theta} = \{\Theta_{ln}\} = \Theta_l \delta_{ln} \quad (54)$$

$$\underline{\mu}^{(i)} = \{\mu_{kn}^{(i)}\} = \mu_k^{(i)} \delta_{kn} \quad (55)$$

$$\underline{K}^{(i)} = \{K_{kn}^{(i)}\} = K_k^{(i)} \delta_{kn} \quad (56)$$

V. SYSTEM STATE EQUATIONS

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

$$\dot{m}^{(i)} = \dot{m}_W^{(\Gamma)(i)} + \dot{m}_{WF}^{(i)} + \dot{m}_U^{(i)} + \dot{m}_{CK}^{(i)} + \dot{m}_K^{(i)} \quad (57)$$

$$\dot{V}^{(i)} = \underline{M}^{(i)-1} \cdot \left(\underline{F}_T^{(\Gamma)(i)} - \underline{F}_K^{(i)} - \underline{F}_P^{(i)} - \underline{F}_D^{(i)} - \underline{F}_C^{(i)} + \underline{F}_G^{(i)} \right) \quad (58)$$

$$\dot{S} = \dot{S}_Q^{(\Gamma)} + \dot{S}_{QF} + \dot{S}_P + \dot{S}_D + \dot{S}_C - \dot{S}_U - \dot{S}_{CK} + \dot{S}_F \quad (59)$$

The different terms in the system state equations (57) to (59) arise from integrations over the domain volume Ω or the domain boundary Γ . Their definitions are:

$$\dot{m}_W^{(\Gamma)(i)} = \left(\underline{\mu}^{(i)} + \underline{K}^{(i)} \right)^{-1} \cdot \left[- \int_{\Gamma} \underline{w}_p^{(i)} \rho^{(i)} \left(\mu^{(i)} + \kappa^{(i)} \right) \underline{V}^{(i)} \cdot \underline{n} \, d\Gamma \right] \quad (60)$$

$$\dot{m}_{WF}^{(i)} = \left(\underline{\mu}^{(i)} + \underline{K}^{(i)} \right)^{-1} \cdot \left[\int_{\Omega} \rho^{(i)} \left(\mu^{(i)} + \kappa^{(i)} \right) \underline{V}^{(i)} \cdot \underline{\nabla} \underline{w}_p^{(i)} \, d\Omega \right] \quad (61)$$

$$\dot{m}_U^{(i)} = \left(\underline{\mu}^{(i)} + \underline{K}^{(i)} \right)^{-1} \cdot \left[\int_{\Omega} \underline{w}_p^{(i)} \rho^{(i)} \underline{V}^{(i)} \cdot \underline{\nabla} \mu^{(i)} \, d\Omega \right] \quad (62)$$

$$\dot{m}_{CK}^{(i)} = \left(\underline{\mu}^{(i)} + \underline{K}^{(i)} \right)^{-1} \cdot \left[\int_{\Omega} \underline{w}_p^{(i)} C^{(i)} \left(\mu^{(i)} + \kappa^{(i)} \right) \, d\Omega \right] \quad (63)$$

$$\dot{m}_K^{(i)} = \left(\underline{\mu}^{(i)} + \underline{K}^{(i)} \right)^{-1} \cdot \left[\int_{\Omega} \underline{w}_p^{(i)} \rho^{(i)} \underline{V}^{(i)} \cdot \underline{\nabla} \kappa^{(i)} \, d\Omega \right] \quad (64)$$

$$\underline{F}_T^{(\Gamma)(i)} = \int_{\Gamma} \left(\underline{T}^{(i)} \cdot \underline{n} \right) \underline{\varphi}_V^{(i)} \, d\Gamma \quad (65)$$

$$\underline{F}_K^{(i)} = \int_{\Omega} \rho^{(i)} \underline{\nabla} \kappa^{(i)} \underline{\varphi}_V^{(i)} \, d\Omega \quad (66)$$

$$\underline{F}_P^{(i)} = \int_{\Omega} \left(\underline{\nabla} P^{(i)} - \underline{f}^{(i)} \right) \underline{\varphi}_V^{(i)} \, d\Omega \quad (67)$$

$$\underline{F}_D^{(i)} = \int_{\Omega} \underline{T}^{(i)} \cdot \underline{\nabla} \underline{\varphi}_V^{(i)} \, d\Omega \quad (68)$$

$$\underline{F}_C^{(i)} = - \int_{\Omega} C^{(i)} \underline{V}^{(i)} \underline{\varphi}_V^{(i)} \, d\Omega \quad (69)$$

$$\underline{F}_G^{(i)} = \int_{\Omega} \rho^{(i)} \underline{G}^{(i)} \underline{\varphi}_V^{(i)} \, d\Omega \quad (70)$$

$$\dot{S}_Q^{(\Gamma)} = \underline{\Theta}^{-1} \cdot \left\{ - \int_{\Gamma} \underline{w}_s \sum_{i=1}^r \left[\underline{q}^{(i)} + \left(\pi^{(i)} s_v - \mu^{(i)} \rho^{(i)} + \sum_{j=1}^r \mu^{(ij)} \rho^{(j)} \right) \underline{V}^{(i)} \right] \cdot \underline{n} \, d\Gamma \right\} \quad (71)$$

$$\dot{S}_{QF} = \underline{\Theta}^{-1} \cdot \left\{ \int_{\Omega} \underline{\nabla} \underline{w}_s \cdot \sum_{i=1}^r \left[\underline{q}^{(i)} + \left(\pi^{(i)} s_v - \mu^{(i)} \rho^{(i)} + \sum_{j=1}^r \mu^{(ij)} \rho^{(j)} \right) \underline{V}^{(i)} \right] \, d\Omega \right\} \quad (72)$$

$$\dot{S}_F = \underline{\Theta}^{-1} \cdot \left[\int_{\Omega} \underline{w}_s \left(\sum_{i=1}^r \rho^{(i)} \Phi^{(i)} \right) \, d\Omega \right] \quad (73)$$

$$\dot{S}_P = \sum_{i=1}^r \dot{S}_P^{(i)} ; \dot{S}_D = \sum_{i=1}^r \dot{S}_D^{(i)} ; \dot{S}_C = \sum_{i=1}^r \dot{S}_C^{(i)} \quad (74)$$

$$\dot{S}_U = \sum_{i=1}^r \dot{S}_U^{(i)} ; \dot{S}_{CK} = \sum_{i=1}^r \dot{S}_{CK}^{(i)} \quad (75)$$

where:

$$\underline{\dot{S}}_P^{(i)} = \underline{\Theta}^{-1} \cdot \left[\int_{\Omega} \underline{w}_s (\nabla P^{(i)} - f^{(i)}) \cdot \underline{V}^{(i)} d\Omega \right] \quad (76)$$

$$\underline{\dot{S}}_D^{(i)} = \underline{\Theta}^{-1} \cdot \left[\int_{\Omega} \underline{w}_s (\nabla \underline{V}^{(i)} : \underline{\tau}^{(i)}) d\Omega \right] \quad (77)$$

$$\underline{\dot{S}}_C^{(i)} = \underline{\Theta}^{-1} \cdot \left[- \int_{\Omega} \underline{w}_s 2 C^{(i)} \kappa^{(i)} d\Omega \right] \quad (78)$$

$$\underline{\dot{S}}_U^{(i)} = \underline{\Theta}^{-1} \cdot \left[\int_{\Omega} \underline{w}_s \rho^{(i)} \underline{V}^{(i)} \cdot \nabla \underline{\mu}^{(i)} d\Omega \right] \quad (79)$$

$$\underline{\dot{S}}_{CK}^{(i)} = \underline{\Theta}^{-1} \cdot \left[\int_{\Omega} \underline{w}_s C^{(i)} (\underline{\mu}^{(i)} + \underline{\kappa}^{(i)}) d\Omega \right] \quad (80)$$

Although the complete Bond Graph is not shown here, it can be said that the state equations (57) and (59) are represented, in the Bond-Graph terminology, by multibond 0-junctions, in which correspondingly the *i*th-component mass rate nodal vectors and the entropy rate nodal vector are added (see Figs. 3 and 4). Eq. (58) 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. (74) and (75).

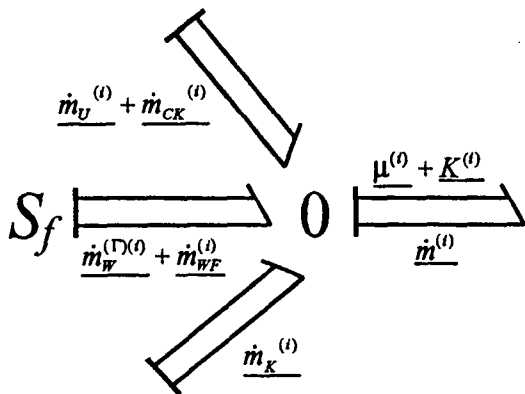


Fig. 3. 0-junction representing the balance equation at the *i*th-component mass port.

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 terms among neighboring nodes. In the discretization procedure, all the terms of the *i*th-component mass balance equation and entropy balance equation were multiplied correspondingly by $\underline{w}_\rho^{(i)}$ and \underline{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-

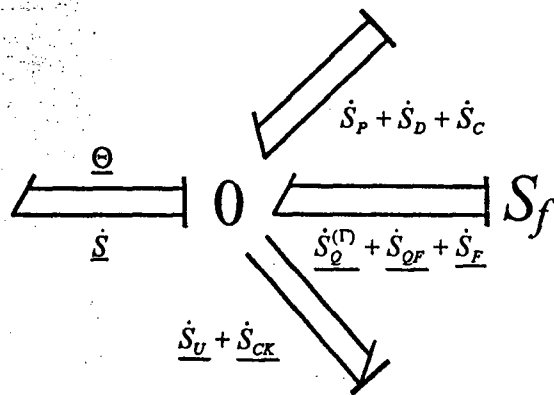


Fig. 4. 0-junction representing the balance equation at the entropy port.

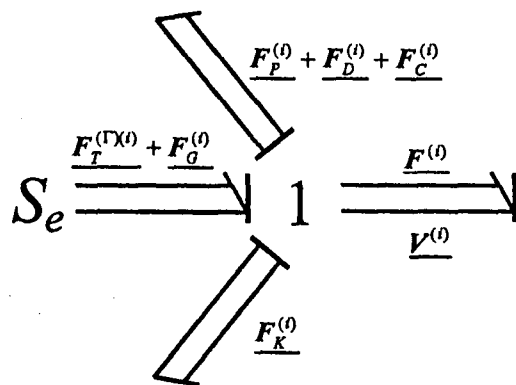


Fig. 5. 1-junction representing the balance equation at the *i*th-component velocity port.

diffusion problems [7][8]. It is very interesting to notice that 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 ($\underline{\dot{m}}_W^{(\Gamma)(i)}$, $\underline{F}_T^{(\Gamma)(i)}$ and $\underline{\dot{S}}_Q^{(\Gamma)}$) and can be represented, in the Bond-Graph terminology, either as generalized modulated effort sources at the inertial ports or modulated flow sources at 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.

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

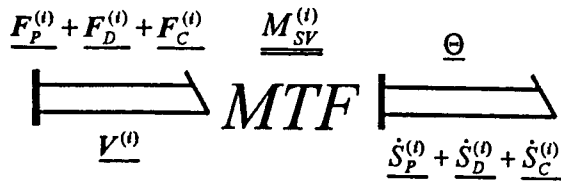


Fig. 6. Power coupling between the *i*th-component velocity and entropy ports.

$$\underline{F}_P^{(i)} + \underline{F}_D^{(i)} + \underline{F}_C^{(i)} = \underline{M}_{SV}^{(i)} \cdot \underline{\Theta} \quad (81)$$

$$\underline{S}_U^{(i)} + \underline{S}_D^{(i)} + \underline{S}_C^{(i)} = \underline{M}_{SV}^{(i)T} \cdot \underline{V}^{(i)} \quad (82)$$

$$\underline{S}_U^{(i)} + \underline{S}_{CK}^{(i)} = \underline{M}_{MS}^{(i)} \cdot (\underline{\mu}^{(i)} + \underline{K}^{(i)}) \quad (83)$$

$$\underline{m}_U^{(i)} + \underline{m}_{CK}^{(i)} = \underline{M}_{MS}^{(i)T} \cdot \underline{\Theta} \quad (84)$$

$$\underline{F}_K^{(i)} = \underline{M}_{MV}^{(i)} \cdot (\underline{\mu}^{(i)} + \underline{K}^{(i)}) \quad (85)$$

$$\underline{m}_K^{(i)} = \underline{M}_{MV}^{(i)T} \cdot \underline{V}^{(i)} \quad (86)$$

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

$$\left\{ \underline{M}_{SV}^{(i)} \right\}_{ml} = \frac{1}{\Theta_l} \int_{\Omega} \left[(\nabla P^{(i)} - \underline{f}^{(i)} - C^{(i)} \underline{V}^{(i)}) \varphi_{Vm}^{(i)} + \underline{T}^{(i)} \cdot \nabla \varphi_{Vm}^{(i)} \right] w_{sl} d\Omega \quad (87)$$

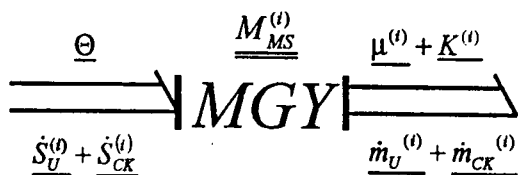


Fig. 7. Power coupling between the *i*th-component entropy and mass ports.



Fig. 8. Power coupling between the *i*th-component velocity and mass ports.

$$\left\{ \underline{M}_{MS}^{(i)} \right\}_{lk} = \frac{1}{\Theta_l} \frac{1}{\mu_k^{(i)} + K_k^{(i)}} \int_{\Omega} \left[\rho^{(i)} \underline{V}^{(i)} \cdot \nabla \mu^{(i)} + C^{(i)} (\mu^{(i)} + \kappa^{(i)}) \right] w_{sl} w_{\rho k}^{(i)} d\Omega \quad (88)$$

$$\left\{ \underline{M}_{MV}^{(i)} \right\}_{mk} = \frac{1}{\mu_k^{(i)} + K_k^{(i)}} \int_{\Omega} \rho^{(i)} \nabla \kappa^{(i)} \varphi_{Vm}^{(i)} d\Omega \quad (89)$$

Since the coupling matrices relate nodal vectors which may have different sizes, they are rectangular and may be not invertible, setting a restriction in the allowable causalities. For instance, from Fig. 6 and Eqs. (81) and (82) it can be seen that the input variables to the ports of the modulated transformer must be $\underline{\Theta}$ and $\underline{V}^{(i)}$, while the output variables result correspondingly the nodal forces and the nodal entropy rates for the *i*th-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 *i*th-component total mass and momentum, as well as the total entropy, is kept constant after the discretization.

VI. DIFFUSION APPROXIMATION

A. Introduction and some definitions

It is common in the literature [9] to describe the dynamics of a multicomponent solution 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 diffusive mass fluxes consist of different contributions associated with the driving forces (mechanical or thermal) existing in the system [10].

In ordinary diffusion, the mass flux depends in a complicated way on the concentration gradients of the components present; in most of the problems, this is the most important contribution.

The pressure diffusion indicates that there may be a differential net movement of a component in the mixture if there is a pressure gradient imposed to the system; this effect is important in centrifuge separation, in which tremendous pressure gradients are established.

The forced diffusion appears when the components are under different external forces, as in the case of ionic systems in presence of electric fields.

Finally, the thermal diffusion describes the tendency for the components to separate under the influence of a temperature gradient. Although this effect is small, it can be enhanced by producing very steep temperature gradients.

Before presenting the diffusion approximation, some definitions of parameters associated to the multicomponent solutions are introduced. The density of the mixture ρ is defined as:

$$\rho = \sum_{i=1}^r \rho^{(i)} \quad (90)$$

Other quantities associated with the mixture can be defined, in order to regard the motion of the solution as a single body. For the case of additive functions, the following definitions are adopted:

$$\rho \mathbf{G} = \sum_{i=1}^r \rho^{(i)} \mathbf{G}^{(i)} ; \rho \Phi = \sum_{i=1}^r \rho^{(i)} \Phi^{(i)} \quad (91)$$

$$\underline{\tau} = \sum_{i=1}^r \underline{\tau}^{(i)} ; \mathbf{q} = \sum_{i=1}^r \mathbf{q}^{(i)} \quad (92)$$

where \mathbf{G} is the body force, Φ is the heat power source per unit mass, $\underline{\tau}$ is the stress and \mathbf{q} is the heat flux corresponding to the mixture.

The average (center of mass) velocity of the mixture \mathbf{V} is defined as:

$$\mathbf{V} = \frac{1}{\rho} \sum_{i=1}^r \rho^{(i)} \mathbf{V}^{(i)} \quad (93)$$

The velocity of the i th-component can be expressed as:

$$\mathbf{V}^{(i)} = \mathbf{V} + \mathbf{v}^{(i)} \quad (94)$$

where $\mathbf{v}^{(i)}$ is the i th-component velocity deviation with respect to the mean velocity. The relative mass flux corresponding to the i th-component $\mathbf{J}^{(i)}$ is defined as:

$$\mathbf{J}^{(i)} = \rho^{(i)} \mathbf{v}^{(i)} \quad (95)$$

From the definition, it is verified that:

$$\sum_{i=1}^r \mathbf{J}^{(i)} = \mathbf{0} \quad (96)$$

In the diffusion approximation, it is assumed that the relative fluxes can be expressed as a function of the thermodynamic state of the system, this is:

$$\mathbf{J}^{(i)} = \mathbf{J}^{(i)}(s_v, \rho^{(1)}, \dots, \rho^{(r)}) \quad (97)$$

This functional dependence allows to deal with ordinary (concentration driven) diffusion, pressure diffusion, forced diffusion (with forces dependent on the thermodynamic state) and thermal diffusion; the corresponding mass fluxes are $\mathbf{J}_C^{(i)}$, $\mathbf{J}_P^{(i)}$, $\mathbf{J}_G^{(i)}$ and $\mathbf{J}_T^{(i)}$, resulting:

$$\mathbf{J}^{(i)} = \mathbf{J}_C^{(i)} + \mathbf{J}_P^{(i)} + \mathbf{J}_G^{(i)} + \mathbf{J}_T^{(i)} \quad (98)$$

The formulas for these flux contributions are [10]:

$$\mathbf{J}_C^{(i)} = \frac{c^2}{\rho R \theta} \sum_{j=1}^r M^{(i)} M^{(j)} D^{(ij)} x^{(j)} \times \sum_{\substack{k=1 \\ k \neq j}}^r \left(\frac{\partial \psi^{(j)}}{\partial x^{(k)}} \right)_{\theta, P, x^{(i \neq j, k)}} \nabla x^{(k)} \quad (99)$$

$$\mathbf{J}_P^{(i)} = \frac{c^2}{\rho R \theta} \sum_{j=1}^r M^{(i)} M^{(j)} D^{(ij)} x^{(j)} M^{(j)} \left(\frac{\overline{v^{(j)}}}{M^{(j)}} - \frac{1}{\rho} \right) \nabla P \quad (100)$$

$$\mathbf{J}_G^{(i)} = -\frac{c^2}{\rho R \theta} \sum_{j=1}^r M^{(i)} M^{(j)} D^{(ij)} x^{(j)} M^{(j)} (\mathbf{G}^{(j)} - \mathbf{G}) \quad (101)$$

$$\mathbf{J}_T^{(i)} = -D_T^{(i)} \frac{\nabla \theta}{\theta} \quad (102)$$

In these equations, R is the gas constant, $\overline{\psi^{(i)}}$ and $\overline{v^{(i)}}$ are respectively the partial molal Gibbs free energy and volume, $M^{(i)}$ is the molecular weight and $x^{(i)}$ is the mole fraction for the i th-component. The mole fraction is calculated as:

$$x^{(i)} = \frac{c^{(i)}}{c} \quad (103)$$

where $c^{(i)}$ is the molar concentration for the i th-component and c is the total molar concentration, defined as:

$$c^{(i)} = \frac{\rho^{(i)}}{M^{(i)}} ; c = \sum_{i=1}^r c^{(i)} \quad (104)$$

The $D^{(ij)}$ are multicomponent diffusion coefficients and the $D_T^{(i)}$ are thermal diffusion coefficients, with the following properties:

$$D^{(ii)} = 0 \quad (105)$$

$$\sum_{i=1}^r \left(M^{(i)} M^{(j)} D^{(ij)} - M^{(i)} M^{(k)} D^{(ik)} \right) = 0 \quad (106)$$

$$\sum_{i=1}^r D_T^{(i)} = 0 \quad (107)$$

B. Kinetic Coenergy per Unit Volume

The main difference between the multivelocity and the diffusion model is the way the kinetic coenergy of the components is taken into account. Since the velocity deviations are functions of the thermodynamic state, the set of state variables corresponding to the inertial ports reduces to the mean velocity. Taking into account Eqs. (94) to (96), the kinetic energy per unit volume can be written as:

$$t_v^* = t_v^* \left(\mathbf{V}, s_v, \rho^{(1)}, \dots, \rho^{(r)} \right) = \frac{1}{2} \rho V^2 + \sum_{i=1}^r \frac{\mathbf{J}^{(i)2}}{2 \rho^{(i)}} \quad (108)$$

The following potentials are defined:

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$$\kappa + \xi^{(i)} = \left(\frac{\partial t_v^*}{\partial \rho^{(i)}} \right)_{V, s_v, \rho^{(j \neq i)}} \quad (109)$$

$$p_v = \left(\frac{\partial t_v^*}{\partial V} \right)_{s_v, \rho^{(j)}} = \rho V \quad (110)$$

$$\zeta = \left(\frac{\partial t_v^*}{\partial s_v} \right)_{V, \rho^{(j)}} = \sum_{j=1}^r \frac{J^{(j)}}{\rho^{(j)}} \cdot \frac{\partial J^{(j)}}{\partial s_v} \quad (111)$$

where:

$$\kappa = \frac{1}{2} V^2 \quad (112)$$

$$\xi^{(i)} = -\frac{J^{(i)2}}{2 \rho^{(i)2}} + \sum_{j=1}^r \frac{J^{(j)}}{\rho^{(j)}} \cdot \frac{\partial J^{(j)}}{\partial \rho^{(i)}} \quad (113)$$

From the definition, the potential $\xi^{(i)}$ is the contribution of the diffusion fluxes to the i th-component kinetic coenergy per unit mass, while ζ can be regarded as a linkage between the mechanical and thermal ports. Notice that p_v results the linear momentum of the mixture. The time derivative of the kinetic coenergy per unit volume can be written as:

$$\frac{\partial t_v^*}{\partial t} = p_v \cdot \frac{\partial V}{\partial t} + \zeta \frac{\partial s_v}{\partial t} + \sum_{i=1}^r (\kappa + \xi^{(i)}) \frac{\partial \rho^{(i)}}{\partial t} \quad (114)$$

C. Total Energy per Unit Volume

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

$$e^* = u_v + t_v^* \quad (115)$$

The representation of the internal energy is the same as in Section II-A. The time derivative of the total energy per unit volume can be written as:

$$\frac{\partial e_v^*}{\partial t} = p_v \cdot \frac{\partial V}{\partial t} + (\theta + \zeta) \frac{\partial s_v}{\partial t} + \sum_{i=1}^r (\mu^{(i)} + \kappa + \xi^{(i)}) \frac{\partial \rho^{(i)}}{\partial t} \quad (116)$$

The potentials defined for the diffusion approximation also satisfy both constitutive and Maxwell relations.

D. Diffusion Balance Equations

Starting from the conservation equations for each component, the mass, momentum and energy conservation equations corresponding to the mixture can be expressed as:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho V) \quad (117)$$

$$\rho \frac{\partial V}{\partial t} = -\sum_{i=1}^r \nabla \cdot (\rho^{(i)} V^{(i)} V^{(i)}) + \nabla \cdot (\rho V V) - \rho V \cdot \nabla V - \nabla P + \sum_{i=1}^r (\nabla \cdot \underline{\underline{T}}^{(i)} + \rho^{(i)} G^{(i)}) \quad (118)$$

$$\frac{\partial u_v}{\partial t} = \sum_{i=1}^r \left[-\nabla \cdot (u_v^{(i)} V^{(i)}) + C^{(i)} \frac{1}{2} V^{(i)2} - P^{(i)} \nabla \cdot V^{(i)} - f^{(i)} \cdot V^{(i)} + \underline{\underline{T}}^{(i)} : \nabla V^{(i)} + \rho^{(i)} \Phi^{(i)} - \nabla \cdot q^{(i)} \right] \quad (119)$$

It can be seen that the non-linear terms appearing in Eqs. (118) and (119) give raise to additional terms in the conservation equations, when compared to the ones corresponding to a single component. As a consequence, the conservation equations for the mixture are not the same as the equations for a single continuum. This conclusion disagrees with many textbooks [5][10].

Taking into account the conservation equations presented in Section III, the mixture conservation equations, the constitutive relations and the diffusion approximation, the balance equations result:

$$\begin{aligned} (\mu^{(i)} + \kappa + \xi^{(i)}) \frac{\partial \rho^{(i)}}{\partial t} = & -\nabla \cdot [(\mu^{(i)} + \kappa) (\rho^{(i)} V + J^{(i)})] \\ & + (\rho^{(i)} V + J^{(i)}) \cdot \nabla \kappa + (\rho^{(i)} V + J^{(i)}) \cdot \nabla \mu^{(i)} \\ & + C^{(i)} (\mu^{(i)} + \kappa + \xi^{(i)}) - \xi^{(i)} \nabla \cdot (\rho^{(i)} V + J^{(i)}) \end{aligned} \quad (120)$$

$$\begin{aligned} p_v \cdot \frac{\partial V}{\partial t} = & \nabla \cdot \left[\underline{\underline{T}} \cdot V - \sum_{i=1}^r \frac{1}{\rho^{(i)}} (J^{(i)} \cdot V) J^{(i)} \right] \\ & - V \cdot \nabla P - \underline{\underline{T}} : \nabla V - \sum_{i=1}^r \rho^{(i)} V \cdot \nabla \kappa + \rho G \cdot V \end{aligned} \quad (121)$$

$$\begin{aligned} (\theta + \zeta) \frac{\partial s_v}{\partial t} = & \nabla \cdot \left\{ -\theta s_v V - q + \sum_{i=1}^r \left[\frac{1}{\rho^{(i)}} \underline{\underline{T}}^{(i)} \cdot J^{(i)} \right. \right. \\ & \left. \left. - \frac{J^{(i)2}}{2 \rho^{(i)}} V - \frac{1}{\rho^{(i)}} \left(\pi^{(i)} s_v - \rho^{(i)} \mu^{(i)} + \sum_{j=1}^r \mu^{(j)} \rho^{(j)} \right) \right. \right. \\ & \left. \left. + \frac{J^{(i)2}}{2 \rho^{(i)}} J^{(i)} \right] \right\} + V \cdot \nabla P + \underline{\underline{T}} : \nabla V \\ & - \sum_{i=1}^r \left[(\rho^{(i)} V + J^{(i)}) \cdot \nabla \mu^{(i)} - \xi^{(i)} \nabla \cdot (\rho^{(i)} V + J^{(i)}) \right. \\ & \left. + C^{(i)} (\mu^{(i)} + \xi^{(i)}) \right] + \sum_{i=1}^r G^{(i)} \cdot J^{(i)} + \rho \Phi \end{aligned} \quad (122)$$

As in the multiveLOCITY model, the balance equations for the diffusion model represent the power structure of the system. Concerning the constitutive and closure laws needed to model a multicomponent solution, it can be observed that in the diffusion model it is not necessary to know the momentum interaction terms between components. It is also interesting to notice the way the divergence and source terms split among the different ports. For instance, the power term corresponding to the stress state splits in two: a term considering the total stress and the mean velocity (influencing the velocity port) and power

terms considering the stress state and the velocity deviations for the different components (influencing the entropy port). A similar behavior can be found for the power term corresponding to the body force and the kinetic coenergy.

The discretization of the balance equations and the resulting Bond Graph for the diffusion model is not shown here, but it is performed in a similar way as in the multivelocity model.

VII. MIXTURE OF IDEAL GASES

As an application example, the potentials defined in Section II-A are calculated for a multicomponent solution (mixture) of ideal gases. The entropic representation of the internal energy for an ideal gas is [6]:

$$u_v^{(i)} = \frac{\rho^{(i)}}{\rho_0} u_{v0}^{(i)} + \rho^{(i)} \int_{\theta_0}^{\theta} c_v^{(i)}(\theta') d\theta' \quad (123)$$

$$s_v = \sum_{i=1}^r \left[\frac{\rho^{(i)}}{\rho_0} s_{v0}^{(i)} + \rho^{(i)} \int_{\theta_0}^{\theta} \frac{c_v^{(i)}(\theta')}{\theta'} d\theta' + \rho^{(i)} R \ln \left(\frac{\rho_0}{\rho^{(i)}} \right) \right] \quad (124)$$

where R is a universal constant, ρ_0 and θ_0 are correspondingly the density and temperature at a reference state, $u_{v0}^{(i)}$ and $s_{v0}^{(i)}$ are the internal energy per unit volume and entropy per unit volume for the i th-component at the reference state and $c_v^{(i)}$ is the i th-component specific heat at constant volume (function of temperature only). Eqs. (123) and (124) are a representation of Eq. (5) in parametric form, being the parameter the temperature θ . From this representation, the potentials result:

$$\pi^{(i)} = \theta \frac{\rho^{(i)} c_v^{(i)}}{\left(\sum_{j=1}^r \rho^{(j)} c_v^{(j)} \right)} \quad (125)$$

$$\begin{aligned} \mu^{(ij)} = & \left(\frac{u_{v0}^{(i)}}{\rho_0} + \int_{\theta_0}^{\theta} c_v^{(i)}(\theta') d\theta' \right) \delta_{ij} \\ & - \theta \frac{\rho^{(i)} c_v^{(i)}}{\left(\sum_{k=1}^r \rho^{(k)} c_v^{(k)} \right)} \left[\frac{s_{v0}^{(j)}}{\rho_0} + \int_{\theta_0}^{\theta} \frac{c_v^{(j)}(\theta')}{\theta'} d\theta' \right. \\ & \left. + R \ln \left(\frac{\rho_0}{\rho^{(j)}} \right) - R \right] \quad (126) \end{aligned}$$

$$P^{(i)} = P \frac{\rho^{(i)} c_v^{(i)}}{\left(\sum_{j=1}^r \rho^{(j)} c_v^{(j)} \right)} \quad (127)$$

where the total pressure results:

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

From Eqs. (125) and (127), it can be seen that the contributions to the total temperature and pressure from the i th-component are weighted by the product of the density and the specific heat.

VIII. CONCLUSIONS

In this paper, the BG-CFD methodology was extended to Multicomponent Solutions. A multivelocity and a diffusion model were presented. 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. 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, two fields that have been following almost separate paths until now. It is hoped that the findings of this paper encourage other researchers to use this formalism in other problems.

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