BG-CFD Methodology for Multicomponent Solutions. Part II: Diffusion Model

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Abstract— **Based on the multivelocity model described in a companion paper submitted to this Conference, a diffusion model 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 with elements of numerical methods. In a companion paper [4], this methodology was extended to multicomponent solution systems [5] in which the component velocities are part of the set of state variables.

It is common in the literature [6] 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 [7].

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.

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 (with steady forces) and thermal diffusion [7].

Unless stated, the reader is referred to the companion paper [4] for the nomenclature adopted here.

II. INDEPENDENT VARIABLES AND POTENTIALS

A. *Diffusion approximation*

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:

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

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:

$$\rho G = \sum_{i=1}^{r} \rho^{(i)} G^{(i)} \quad ; \quad \rho \Phi = \sum_{i=1}^{r} \rho^{(i)} \Phi^{(i)} \tag{2}$$

$$\underline{\underline{\tau}} = \sum_{i=1}^{r} \underline{\underline{\tau}}^{(i)} \quad ; \quad q = \sum_{i=1}^{r} q^{(i)} \tag{3}$$

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

The average (center of mass) velocity of the mixture V is defined as:

$$V = \frac{1}{\rho} \sum_{i=1}^{r} \rho^{(i)} V^{(i)} \tag{4}$$

The velocity of the ith-component can be expressed as:

$$V^{(i)} = V - v^{(i)} \tag{5}$$

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

$$J^{(i)} = \rho^{(i)} v^{(i)} \tag{6}$$

From the definition, it is verified that:

$$\sum_{i=1}^{r} J^{(i)} = 0 \tag{7}$$

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:

$$J^{(i)} = J^{(i)} \left(s_v, \rho^{(1)}, ..., \rho^{(r)} \right) \tag{8}$$

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 $J_C^{(i)}$, $J_P^{(i)}$, $J_G^{(i)}$ and $J_T^{(i)}$, resulting:

$$J^{(i)} = J_C^{(i)} + J_P^{(i)} + J_G^{(i)} + J_T^{(i)} \tag{9}$$

The formulas for these flux contributions are [7]:

$$J_C^{(i)} = \frac{c^2}{\rho R\theta} \sum_{j=1}^{r} M^{(i)} M^{(j)} D^{(ij)} x^{(j)} \times \sum_{\substack{k=1 \\ k\neq j}}^{r} \left(\frac{\partial \overline{\psi^{(j)}}}{\partial x^{(k)}} \right)_{\theta, P, x(a\neq j,\, k)} \nabla x^{(k)} \tag{10}$$

$$J_P^{(i)} = \frac{c^2}{\rho R\theta} \sum_{j=1}^{r} M^{(i)} M^{(j)} D^{(ij)} x^{(j)} M^{(j)} \left(\frac{\overline{v^{(j)}}}{M^{(j)}} - \frac{1}{\rho} \right) \nabla P \tag{11}$$

$$J_G^{(i)} = -\frac{c^2}{\rho R\theta} \sum_{j=1}^{r} M^{(i)} M^{(j)} D^{(ij)} x^{(j)} M^{(j)} \left(G^{(j)} - G \right) \tag{12}$$

$$J_T^{(i)} = -D_T^{(i)} \frac{\nabla\theta}{\theta} \tag{13}$$

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 ith-component. The mole fraction is calculated as:

$$x^{(i)} = \frac{c^{(i)}}{c} \tag{14}$$

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

$$c^{(i)} = \frac{\rho^{(i)}}{M^{(i)}} \quad ; \quad c = \sum_{i=1}^{r} c^{(i)} \tag{15}$$

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

$$D^{(ii)} = 0 \tag{16}$$

$$\sum_{i=1}^{r} \left(M^{(i)} M^{(j)} D^{(ij)} - M^{(i)} M^{(k)} D^{(ik)} \right) = 0 \tag{17}$$

$$\sum_{i=1}^{r} D_T^{(i)} = 0 \tag{18}$$

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. (5) to (7), the kinetic energy per unit volume can be written as:

$$t_v^* = t_v^* \left(\boldsymbol{V}, s_v, \rho^{(1)}, \ldots, \rho^{(r)} \right) = \frac{1}{2} \rho \boldsymbol{V}^2 + \sum_{i=1}^{r} \frac{\boldsymbol{J}^{(i)2}}{2\,\rho^{(i)}} \tag{19}$$

The following potentials are defined:

$$\kappa - \xi^{(i)} = \left(\frac{\partial t_v^*}{\partial \rho^{(i)}} \right)_{\boldsymbol{V}, s_v, \rho^{(j\neq i)}} \tag{20}$$

$$\boldsymbol{p}_v = \left(\frac{\partial t_v^*}{\partial \boldsymbol{V}} \right)_{s_v, \rho^{(j)}} = \rho \boldsymbol{V} \tag{21}$$

$$\zeta = \left(\frac{\partial t_v^*}{\partial s_v} \right)_{\boldsymbol{V}, \rho^{(j)}} = \sum_{j=1}^{r} \frac{\boldsymbol{J}^{(j)}}{\rho^{(j)}} \cdot \frac{\partial \boldsymbol{J}^{(j)}}{\partial s_v} \tag{22}$$

where:

$$\kappa = \frac{1}{2} \boldsymbol{V}^2 \tag{23}$$

$$\xi^{(i)} = -\frac{\boldsymbol{J}^{(i)2}}{2\,\rho^{(i)2}} + \sum_{j=1}^{r} \frac{\boldsymbol{J}^{(j)}}{\rho^{(j)}} \cdot \frac{\partial \boldsymbol{J}^{(j)}}{\partial \rho^{(i)}} \tag{24}$$

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

$$\frac{\partial t_v^*}{\partial t} = \boldsymbol{p}_v \cdot \frac{\partial \boldsymbol{V}}{\partial t} + \zeta \frac{\partial s_v}{\partial t} + \sum_{i=1}^{r} \kappa^{(i)} \frac{\partial \rho^{(i)}}{\partial t} \tag{25}$$

C. Total Energy per Unit Volume

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

$$e_v^* = u_v + t_v^* \tag{26}$$

The representation of the internal energy is the same as in [4]. The time derivative of the total energy per unit volume can be written as:

$$\frac{\partial e_v^*}{\partial t} = \boldsymbol{p}_v \cdot \frac{\partial \boldsymbol{V}}{\partial t} + (\theta + \zeta) \frac{\partial s_v}{\partial t} + \sum_{i=1}^{r} \left(\mu^{(i)} - \kappa - \xi^{(i)} \right) \frac{\partial \rho^{(i)}}{\partial t} \tag{27}$$

As in [4], the potentials multiplying the time derivatives of the independent variables satisfy both constitutive and Maxwell relations [8].

III. 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:

$$\frac{\partial \rho}{\partial t} = -\nabla . (\rho \boldsymbol{V}) \tag{28}$$

$$\rho \frac{\partial \boldsymbol{V}}{\partial t} = -\sum_{i=1}^{r} \nabla . \left(\rho^{(i)} \boldsymbol{V}^{(i)} \boldsymbol{V}^{(i)} \right) + \nabla . (\rho \boldsymbol{V} \boldsymbol{V}) - \rho \boldsymbol{V} . \nabla \boldsymbol{V} - \nabla P + \nabla . \underline{\underline{\tau}} + \rho \boldsymbol{G} \tag{29}$$

$$\frac{\partial u_v}{\partial t} = \sum_{i=1}^{r} \left[-\nabla . \left(u_v^{(i)} \boldsymbol{V}^{(i)} \right) + C^{(i)} \frac{1}{2} \boldsymbol{V}^{(i)2} - P^{(i)} \nabla . \boldsymbol{V}^{(i)} - \boldsymbol{f}^{(i)} . \boldsymbol{V}^{(i)} + \underline{\underline{\tau}}^{(i)} : \nabla \boldsymbol{V}^{(i)} \right] - \rho \Phi - \nabla . q \tag{30}$$

It can be seen that the non-linear terms appearing in Eqs. (29) and (30) 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][7].

Taking into account the conservation equations presented in [4], the mixture conservations equations, the constitutive relations and the diffusion approximation, the balance equations result:

$$\left(\mu^{(i)}+\kappa+\xi^{(i)}\right)\frac{\partial \rho^{(i)}}{\partial t}=-\nabla.\left[\left(\mu^{(i)}+\kappa\right)\left(\rho^{(i)}\,V+J^{(i)}\right)\right]$$
$$+\left(\rho^{(i)}\,V+J^{(i)}\right).\nabla\kappa+\left(\rho^{(i)}\,V+J^{(i)}\right).\nabla\mu^{(i)}$$
$$+C^{(i)}\left(\mu^{(i)}+\kappa+\xi^{(i)}\right)-\xi^{(i)}\,\nabla.\left(\rho^{(i)}\,V+J^{(i)}\right) \quad (31)$$

$$p_v.\frac{\partial \boldsymbol{V}}{\partial t}=\nabla.\left[\underline{\underline{\tau}}.V-\sum_{i=1}^{r}\frac{1}{\rho^{(i)}}\left(J^{(i)}.V\right)J^{(i)}\right]$$
$$-V.\nabla P-\underline{\underline{\tau}}:\nabla V-\rho\,V.\nabla\kappa+\rho\,G.V \quad (32)$$

$$(\theta+\zeta)\frac{\partial s_v}{\partial t}=\nabla.\left\{-\theta\,s_v\,V-q+\sum_{i=1}^{r}\left[\frac{1}{\rho^{(i)}}\underline{\underline{\tau^{(i)}}}.J^{(i)}\right.\right.$$
$$-\frac{J^{(i)2}}{2\,\rho^{(i)}}V-\frac{1}{\rho^{(i)}}\left(\pi^{(i)}\,s_v-\rho^{(i)}\,\mu^{(i)}+\sum_{j=1}^{r}\mu^{(ij)}\,\rho^{(j)}\right.$$
$$\left.\left.\left.+\frac{J^{(i)2}}{2\,\rho^{(i)}}\right)J^{(i)}\right]\right\}+V.\nabla P+\underline{\underline{\tau}}:\nabla V$$
$$-\sum_{i=1}^{r}\left[\left(\rho^{(i)}\,V+J^{(i)}\right).\nabla\mu^{(i)}-\xi^{(i)}\,\nabla.\left(\rho^{(i)}\,V+J^{(i)}\right)\right.$$
$$\left.+C^{(i)}\left(\mu^{(i)}+\xi^{(i)}\right)\right]+\sum_{i=1}^{r}G^{(i)}.J^{(i)}+\rho\,\Phi \quad (33)$$

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 diffusive fluxes 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. Taking into account Eq. (27) it verifies that coupling terms cancel out when the balance equations are added, resulting:

$$\frac{\partial e_v^*}{\partial t}=-\nabla.\left[\left(u_v-P+\rho\kappa-\sum_{i=1}^{r}\frac{J^{(i)2}}{2\,\rho^{(i)}}\right)V\right]$$
$$-\sum_{i=1}^{r}\nabla.\left[\frac{1}{\rho^{(i)}}\left(u_v^{(i)}+P^{(i)}-\frac{J^{(i)2}}{2\,\rho^{(i)}}\right)J^{(i)}\right]$$
$$+\nabla.\left(\underline{\underline{\tau}}.V\right)-\sum_{i=1}^{r}\nabla.\left(\frac{1}{\rho^{(i)}}\underline{\underline{\tau^{(i)}}}.J^{(i)}\right)-\nabla.q^{(i)}$$
$$+\rho\,G.V-\sum_{i=1}^{r}G^{(i)}.J^{(i)}+\rho\,\Phi \quad (34)$$

IV. DISCRETIZATION

The discretization for the component densities and for the entropy per unit volume remain the same as in the multivelocity model. For the velocity field, we have:

$$\boldsymbol{V}(r,t)=\sum_{m=1}^{nV}V_m(t)\,\varphi_{Vm}(r)=\underline{V}^T.\underline{\varphi_V} \quad (35)$$

The system kinetic coenergy, with the diffusion approximation, results:

$$T^*=T^*\left(\underline{V},\underline{S},\underline{m^{(1)}},...,\underline{m^{(r)}}\right)=\int_\Omega\left(\frac{1}{2}\rho\,V^2-\sum_{i=1}^{r}\frac{J^{(i)2}}{2\,\rho^{(i)}}\right)d\Omega \quad (36)$$

The integrated potentials are:

$$\underline{p}=\left(\frac{\partial T^*}{\partial \underline{V}}\right)_{\underline{S},\underline{m^{(i)}}}=\underline{\underline{M}}.\underline{V}=\int_\Omega p_v\,\underline{\varphi_V}\,d\Omega \quad (37)$$

$$\underline{\zeta}=\left(\frac{\partial T^*}{\partial \underline{S}}\right)_{\underline{V},\underline{m^{(i)}}}=\underline{\underline{\Omega_s}}^{-1}.\left[\int_\Omega\zeta\,\underline{\varphi_s}\,d\Omega\right] \quad (38)$$

$$\underline{K^{(i)}}+\underline{\xi^{(i)}}=\left(\frac{\partial T^*}{\partial \underline{m^{(i)}}}\right)_{\underline{V},\underline{S},\underline{m^{(j\neq i)}}} \quad (39)$$

where:

$$\underline{K^{(i)}}=\underline{\underline{\Omega_\rho^{(i)}}}^{-1}.\left[\int_\Omega\kappa\,\underline{\varphi_\rho^{(i)}}\,d\Omega\right] \quad (40)$$

$$\underline{\xi^{(i)}}=\underline{\underline{\Omega_\rho^{(i)}}}^{-1}.\left[\int_\Omega\xi^{(i)}\,\underline{\varphi_\rho^{(i)}}\,d\Omega\right] \quad (41)$$

The inertia matrix introduced in Eq. (37) is defined as:

$$\underline{\underline{M}}=\{M\}_{mn}=\int_\Omega\rho\,\varphi_{Vm}\,\varphi_{Vn}\,d\Omega \quad (42)$$

Eq. (37) defines, in the Bond-Graph terminology, a modulated multibond transformer relating the nodal vectors of mixture 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 [9]. According to the power conservation across the transformer, the generalized effort is given by:

$$\underline{F}=\underline{\underline{M}}.\dot{\underline{V}} \quad (43)$$

Fig. 1. Modulated inertial transformer.

According to Eq. (37), the nodal vector of mixture linear momentum can be regarded as a system volume integral of the local value weighted by the velocity interpolation function. The system mixture linear momentum can be obtained as:

$$p=\int_\Omega p_v\,d\Omega=\sum_{m=1}^{nV}p_m \quad (44)$$

Introducing the potential coming from the internal energy, the time derivative of the system total energy can be written as:

$$\dot{E}^*=\left(\underline{\Theta}+\underline{\zeta}\right)^T.\dot{\underline{S}}+\underline{p}^T.\dot{\underline{V}}+\sum_{i=1}^{r}\left(\underline{\mu^{(i)}}-\underline{K^{(i)}}-\underline{\xi^{(i)}}\right)^T.\dot{\underline{m^{(i)}}} \quad (45)$$

It can also be shown that the volume integrals of the left side terms of Eqs. (31) to (33) can be calculated as:

$$\int_{\Omega} \left(\mu^{(i)} + \kappa + \xi^{(i)}\right) \frac{\partial \rho^{(i)}}{\partial t}\, d\Omega = \left(\underline{\mu^{(i)}} - \underline{K^{(i)}} + \underline{\xi^{(i)}}\right)^{T} . \underline{\dot{m}^{(i)}} \tag{46}$$

$$\int_{\Omega} \boldsymbol{p}_v . \frac{\partial \mathbf{V}}{\partial t}\, d\Omega = \underline{p}^{T} . \underline{\dot{V}} \tag{47}$$

$$\int_{\Omega} (\theta + \zeta) \frac{\partial s_v}{\partial t}\, d\Omega = (\underline{\Theta} - \underline{\zeta})^{T} . \underline{\dot{S}} \tag{48}$$

As in the multivelocity model, the representation of the total energy as a function of the state variables $\underline{S}$, $\underline{\mathbf{V}}$ and $\underline{m^{(i)}}$ define, in the Bond-Graph terminology, a multibond IC-field associated to the system total energy, as shown in Fig. 2. This field has one inertial port (the velocity port) and $r+1$ capacitive ports (the entropy port and the r mass ports). The generalized effort variables associated to these ports are $\underline{\dot{V}}$, $(\underline{\Theta} + \underline{\zeta})$ and $\left(\underline{\mu^{(i)}} + \underline{K^{(i)}} + \underline{\xi^{(i)}}\right)$, while the generalized flow variables are correspondingly $\underline{p}$, $\underline{\dot{S}}$ and $\underline{\dot{m}^{(i)}}$.

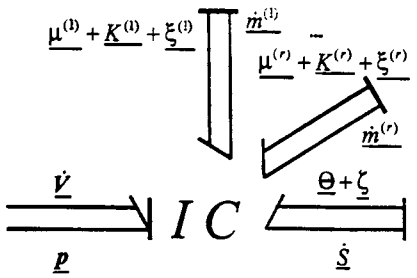

Fig. 2. System IC-field for the diffusion model.

For the sake of convenience, we also define the following diagonal matrices:

$$\underline{\zeta} = \{\zeta\}_{ln} = \zeta_l\, \delta_{ln} \tag{49}$$

$$\underline{\underline{\xi^{(i)}}} = \left\{\xi^{(i)}\right\}_{kn} = \xi_k^{(i)}\, \delta_{kn} \tag{50}$$

V. SYSTEM STATE EQUATIONS

The expressions for the system state equations are:

$$\underline{\dot{m}^{(i)}} = \underline{\dot{m}_W^{(\Gamma)(i)}} - \underline{\dot{m}_{WF}^{(i)}} - \underline{\dot{m}_U^{(i)}} - \underline{\dot{m}_{CK}^{(i)}} - \underline{\dot{m}_K^{(i)}} - \underline{\dot{m}_E^{(i)}} \tag{51}$$

$$\underline{\dot{\mathbf{V}}} = \underline{\underline{M}}^{-1} . \left(\underline{\mathbf{F}_T^{(\Gamma)}} - \underline{F_K} - \underline{F_P} - \underline{F_D} + \underline{\mathbf{F}_G}\right) \tag{52}$$

$$\underline{\dot{S}} = \underline{\dot{S}_Q^{(\Gamma)}} + \underline{\dot{S}_{QF}} + \underline{\dot{S}_P} + \underline{\dot{S}_D} - \underline{\dot{S}_U} - \underline{\dot{S}_{CK}} - \underline{\dot{S}_E} + \underline{\dot{S}_F} \tag{53}$$

The definitions for the different terms in the system state equations are:

$$\underline{\dot{m}_W^{(\Gamma)(i)}} = -\underline{\underline{E_M^{(i)}}} . \left[\int_{\Gamma} \underline{w_\rho^{(i)}} \left(\rho^{(i)}\, \mathbf{V} - \mathbf{J}^{(i)}\right) \left(\mu^{(i)} + \kappa\right) \mathbf{V} . \check{\mathbf{n}}\, d\Gamma\right] \tag{54}$$

$$\underline{\dot{m}_{WF}^{(i)}} = \underline{\underline{E_M^{(i)}}} . \left[\int_{\Omega} \left(\rho^{(i)}\, \mathbf{V} + \mathbf{J}^{(i)}\right) \left(\mu^{(i)} - \kappa\right) \mathbf{V} . \underline{\nabla w_\rho^{(i)}}\, d\Omega\right] \tag{55}$$

$$\underline{\dot{m}_U^{(i)}} = \underline{\underline{E_M^{(i)}}} . \left[\int_{\Omega} \underline{w_\rho^{(i)}} \left(\rho^{(i)}\, \mathbf{V} + \mathbf{J}^{(i)}\right) \nabla \mu^{(i)}\, d\Omega\right] \tag{56}$$

$$\underline{\dot{m}_{CK}^{(i)}} = \underline{\underline{E_M^{(i)}}} . \left[\int_{\Omega} \underline{w_\rho^{(i)}}\, C^{(i)} \left(\mu^{(i)} + \kappa + \xi^{(i)}\right) d\Omega\right] \tag{57}$$

$$\underline{\dot{m}_K^{(i)}} = \underline{\underline{E_M^{(i)}}} . \left[\int_{\Omega} \underline{w_\rho^{(i)}} \left(\rho^{(i)}\, \mathbf{V} + \mathbf{J}^{(i)}\right) \nabla \kappa^{(i)}\, d\Omega\right] \tag{58}$$

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

$$\underline{\mathbf{F}_T^{(\Gamma)}} = \int_{\Gamma} \left[\underline{\underline{\tau}} . \check{\mathbf{n}} - \sum_{i=1}^{r} \int_{\Gamma} \frac{1}{\rho^{(i)}} \left(\mathbf{J}^{(i)} . \check{\mathbf{n}}\right) \mathbf{J}^{(i)}\right] \underline{\varphi_V}\, d\Gamma \tag{60}$$

$$\underline{F_K} = \int_{\Omega} \rho\, \nabla \kappa\, \underline{\varphi_V}\, d\Omega \tag{61}$$

$$\underline{F_P} = \int_{\Omega} \nabla P\, \underline{\varphi_V^{(i)}}\, d\Omega \tag{62}$$

$$\underline{F_D} = \int_{\Omega} \underline{\underline{\tau}} . \nabla \underline{\varphi_V}\, d\Omega \tag{63}$$

$$\underline{F_G} = \int_{\Omega} \rho\, G\, \underline{\varphi_V}\, d\Omega \tag{64}$$

$$\underline{\dot{S}_Q^{(\Gamma)}} = \left(\underline{\underline{\Theta}} + \underline{\underline{\zeta}}\right)^{-1} . \left\langle - \int_{\Gamma} \underline{w_s} \left\{q - \theta\, s_v\, \mathbf{V} + \sum_{i=1}^{r} \left[-\frac{1}{\rho^{(i)}}\, \underline{\underline{\tau^{(i)}}} . \mathbf{J}^{(i)} + \frac{\mathbf{J}^{(i)2}}{2\,\rho^{(i)}}\, \mathbf{V} + \frac{1}{\rho^{(i)}} \left(\pi^{(i)}\, s_v - \rho^{(i)}\, \mu^{(i)} + \sum_{j=1}^{r} \mu^{(ij)}\, \rho^{(j)} - \frac{\mathbf{J}^{(i)2}}{2\,\rho^{(i)}}\right) \mathbf{J}^{(i)}\right]\right\} . \check{\mathbf{n}}\, d\Gamma\right\rangle \tag{65}$$

$$\underline{\dot{S}_{QF}} = \left(\underline{\underline{\Theta}} + \underline{\underline{\zeta}}\right)^{-1} . \left\langle \int_{\Omega} \underline{\nabla w_s} . \left\{q - \theta\, s_v\, \mathbf{V} + \sum_{i=1}^{r} \left[-\frac{1}{\rho^{(i)}}\, \underline{\underline{\tau^{(i)}}} . \mathbf{J}^{(i)} + \frac{\mathbf{J}^{(i)2}}{2\,\rho^{(i)}}\, \mathbf{V} + \frac{1}{\rho^{(i)}} \left(\pi^{(i)}\, s_v - \rho^{(i)}\, \mu^{(i)} + \sum_{j=1}^{r} \mu^{(ij)}\, \rho^{(j)} - \frac{\mathbf{J}^{(i)2}}{2\,\rho^{(i)}}\right) \mathbf{J}^{(i)}\right]\right\} d\Omega\right\rangle \tag{66}$$

$$\underline{\dot{S}_F} = \left(\underline{\underline{\Theta}} + \underline{\underline{\zeta}}\right)^{-1} . \left[\int_{\Omega} \underline{w_s} \left(\rho\, \Phi - \sum_{i=1}^{r} \mathbf{G}^{(i)} . \mathbf{J}^{(i)}\right) d\Omega\right] \tag{67}$$

$$\underline{\dot{S}_P} = \left(\underline{\underline{\Theta}} + \underline{\underline{\zeta}}\right)^{-1} . \left[\int_{\Omega} \underline{w_s} \left(\nabla \mathbf{V} : \underline{\underline{\tau}}\right) d\Omega\right] \tag{68}$$

$$\underline{\dot{S}_D} = \left(\underline{\underline{\Theta}} + \underline{\underline{\zeta}}\right)^{-1} . \left[\int_{\Omega} \underline{w_s} \left(\nabla \mathbf{V} : \underline{\underline{\tau}}\right) d\Omega\right] \tag{69}$$

$$\underline{\dot{S}_{CK}} = \left(\underline{\underline{\Theta}} + \underline{\underline{\zeta}}\right)^{-1} . \left[\int_{\Omega} \underline{w_s} \sum_{i=1}^{r} C^{(i)} \left(\mu^{(i)} - \xi^{(i)}\right) d\Omega\right] \tag{70}$$

$$\underline{\dot{S}_U} = \sum_{i=1}^{r} \underline{\dot{S}_U^{(i)}} \quad ; \quad \underline{\dot{S}_E} = \sum_{i=1}^{r} \underline{\dot{S}_E^{(i)}} \tag{71}$$

where:

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

$$\underline{\dot{S}_U^{(i)}} = \left(\underline{\underline{\Theta}} + \underline{\zeta}\right)^{-1} \cdot \left[\int_\Omega \underline{w_s} \left(\rho^{(i)} \boldsymbol{V} + \boldsymbol{J}^{(i)}\right) . \nabla \mu^{(i)} \, d\Omega\right] \tag{72}$$

$$\underline{\dot{S}_{CK}^{(i)}} = \left(\underline{\underline{\Theta}} + \underline{\zeta}\right)^{-1} \cdot \left[\int_\Omega \underline{w_s} \xi^{(i)} \nabla . \left(\rho^{(i)} \boldsymbol{V} + \boldsymbol{J}^{(i)}\right) d\Omega\right] \tag{73}$$

It can be shown that Eqs. (61) and (70) can be obtained as:

$$\underline{\boldsymbol{F}_K} = \sum_{i=1}^{r} \underline{\boldsymbol{F}_K^{(i)}} \quad ; \quad \underline{\dot{S}_{CK}} = \sum_{i=1}^{r} \underline{\dot{S}_{CK}^{(i)}} \tag{74}$$

where:

$$\underline{\boldsymbol{F}_K^{(i)}} = \int_\Omega \left[\rho^{(i)} \nabla \kappa + \boldsymbol{J}^{(i)} . \nabla \boldsymbol{V}^T - \boldsymbol{J}^{(i)} \times (\nabla \times \boldsymbol{V})\right] \underline{\varphi_V} \, d\Omega \tag{75}$$

$$\underline{\dot{S}_{CK}^{(i)}} = \left(\underline{\underline{\Theta}} + \underline{\zeta}\right)^{-1} \cdot \left[\int_\Omega \underline{w_s} C^{(i)} \left(\mu^{(i)} + \kappa + \xi^{(i)}\right) d\Omega\right] \tag{76}$$

Although the complete Bond Graph is not shown here, it can be said that the state equations (51) and (53) 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. (52) is represented, in the Bond-Graph terminology, by a multibond 1-junction, in which the forces are added (see Fig. 5). Multibond 0-junctions are also used to represent Eqs. (71) and (74).

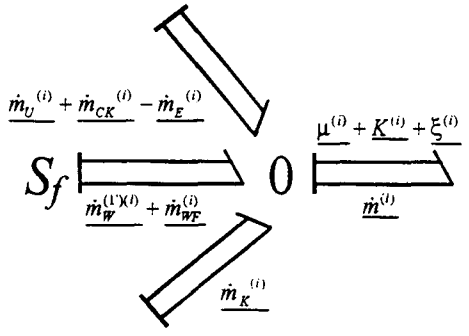

Fig. 3. 0-junction representing the balance equation at the ith-component mass port.

The density and entropy weight functions $\underline{w_\rho^{(i)}}$ and $\underline{w_s}$ are introduced as in the multivelocity model. The boundary conditions and initial conditions are also handled analogously through generalized modulated effort sources at the inertial port or modulated flow sources at the capacitive ports, as shown in Figs. 3 to 5.

The discretized representation of the power couplings are also represented by 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:

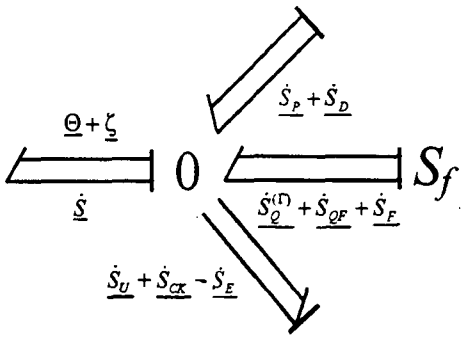

Fig. 4. 0-junction representing the balance equation at the entropy port.

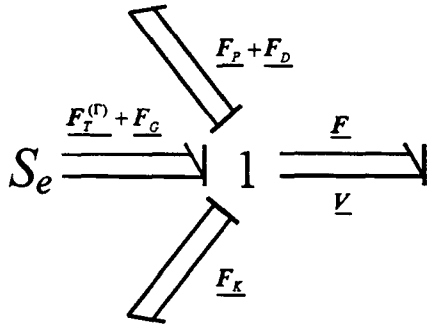

Fig. 5. 1-junction representing the balance equation at the velocity port.

$$\underline{\boldsymbol{F}_P} + \underline{\boldsymbol{F}_D} = \underline{\underline{M_{SV}}} . (\underline{\Theta} + \underline{\zeta}) \tag{77}$$

$$\underline{\dot{S}_P} + \underline{\dot{S}_D} = \underline{\underline{M_{SV}}}^T . \boldsymbol{V} \tag{78}$$

$$\underline{\dot{S}_U^{(i)}} + \underline{\dot{S}_{CK}^{(i)}} - \underline{\dot{S}_E^{(i)}} = \underline{\underline{M_{MS}^{(i)}}} . \left(\underline{\mu^{(i)}} + \underline{K^{(i)}} - \underline{\xi^{(i)}}\right) \tag{79}$$

$$\underline{\dot{m}_U^{(i)}} + \underline{\dot{m}_{CK}^{(i)}} - \underline{\dot{m}_E^{(i)}} = \underline{\underline{M_{MS}^{(i)}}}^T . (\underline{\Theta} + \underline{\zeta}) \tag{80}$$

$$\underline{\boldsymbol{F}_K^{(i)}} = \underline{\underline{M_{MV}^{(i)}}} . \left(\underline{\mu^{(i)}} - \underline{K^{(i)}} + \underline{\xi^{(i)}}\right) \tag{81}$$

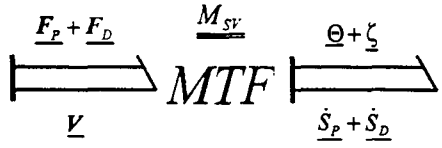

Fig. 6. Power coupling between the velocity and entropy ports.

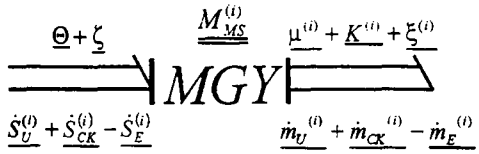

Fig. 7. Power coupling between the ith-component entropy and mass ports.

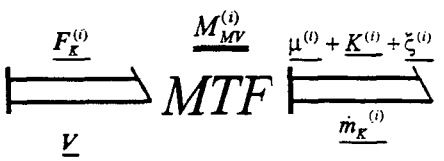

Fig. 8. Power coupling between the velocity and ith-component mass ports.

$$\underline{\dot{m}_K^{(i)}} = \underline{\underline{M_{MV}^{(i)}}}^T \cdot \underline{V} \tag{82}$$

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

$$\left\{\underline{\underline{M_{SV}}}\right\}_{ml} = \frac{1}{\Theta_l + \zeta_l} \int_\Omega \left[\nabla P \varphi_{Vm} + \underline{\underline{\tau}} \cdot \nabla \varphi_{Vm}\right] w_{sl}\, d\Omega \tag{83}$$

$$\left\{\underline{\underline{M_{MS}^{(i)}}}\right\}_{lk} = \frac{1}{\Theta_l + \zeta_l} \frac{1}{\mu_k^{(i)} + K_k^{(i)} + \xi_k^{(i)}} \int_\Omega \left[\left(\rho^{(i)} V + J^{(i)}\right) \nabla \mu^{(i)} + C^{(i)} \left(\mu^{(i)} + \kappa + \xi^{(i)}\right) - \xi^{(i)} \nabla \cdot \left(\rho^{(i)} V + J^{(i)}\right)\right] w_{\rho k}^{(i)} w_{sl}\, d\Omega \tag{84}$$

$$\left\{\underline{\underline{M_{MV}^{(i)}}}\right\}_{mk} = \frac{1}{\mu_k^{(i)} + K_k^{(i)} + \xi_k^{(i)}} \int_\Omega \left[\rho^{(i)} \nabla \kappa + J^{(i)} \cdot \nabla V^T - J^{(i)} \times (\nabla \times V)\right] w_{\rho k}^{(i)} \varphi_{Vm}\, d\Omega \tag{85}$$

As in the multivelocity model, the coupling matrices set restrictions in the allowable causalities.

VI. CONCLUSIONS

Based on the multivelocity model described in a companion paper submitted to this Conference, a diffusion model 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.

The author believes that a methodology such as BG-CFD, based on the representation of the total energy per unit volume and the differential equations coming from Continuum Theory, is the right approach for discretizing continuous systems. The balance equations, which are a original contribution of this methodology, represent the power structure of the system and can take into account all physical effects. Other models encountered in the literature, many of them including discretization assumptions, can be obtained as particular cases.

Finally, it can be said that this methodology can be used in any continuous system in which a power representation and differential conservation equations exist (Solid Mechanics, Electrodynamics, etc.). In the field of Computational Fluid Dynamics, areas of interest for the application of this methodology are Turbulence and Multiphase Flow, in which more sophisticated averaging procedures must be resorted to.

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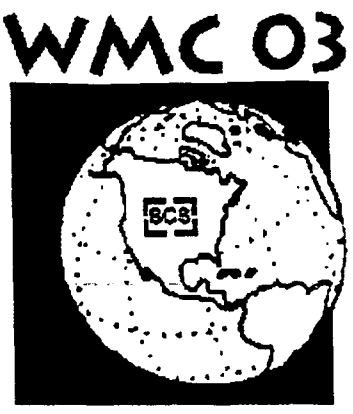

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Errata

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