The Energy Equation in Microchemical Systems

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Microchemical systems gained considerable interest in many areas in engineering and technology. These microchemical systems have gone beyond prototypes and laboratory setups to real life implementation. They are widely used in biological applications as micro total analysis systems (µtas), and in low-to-medium power generation as micro fuel cells [Jensen 1999].

To assess and optimize the performance and functionality of these microchemical systems, adequate models that incorporate the unique phenomena pertinent to microfluidic flows in microchemical processes have to be developed. Fluid dynamics models based on partial differential equations will become more complicated [Alfadhel and Kothare 2004-1] and perhaps unsolvable [Lockerby and Reese 2000] when one considers secondary phenomena such as velocity-slip on the walls of the microchannels. Due to size reduction, thus higher Knudsen number (Kn), the continuum assumption may be violated [Xue et al. 2001]. Continuum approaches based on Navier-Stokes equations are applicable only when Kn < 0.1 although the continuum assumption upholds above that limit [Gad-el-Hak 2003]. The no-velocity-slip/no-temperature-jump boundary conditions require a more stringent criterion [Arkilic et al. 1997, Cai et al. 2000, Jie et al. 2000].

Mass and heat transfer models involve higher level of complexity when written for microchemical processes. It is not only that rigorous models for this class of systems do not exist in the literature; the modification of the boundary conditions to relax the existing models to capture the physics of microchemical systems remains an area of on-going research. In an earlier work, we developed analytical mathematical models for flow in microchannels incorporating membrane permeation [Alfadhel and Kothare 2004-1], and proposed an alternative modeling approach to the multicomponent mass balance problem in membrane microreactors [Alfadhel and Kothare 2004-2].

To obtain the energy equation for multicomponent systems, one has to include the energy exchange due to the diffusion of different species having dissimilar partial molar

enthalpies, H_i. Also, one has to allow for the diffusion thermo effect (Dufour Effect), $q^{(x)}$, and the possibility of having other body forces different from gravity. We start from the energy equation for single component,

$$\rho \frac{D}{Dt}\left(U + \frac{v^2}{2}\right) = -\nabla \cdot q + \rho(v \cdot g) - \nabla \cdot (Pv) + \nabla \cdot (\tau \cdot v) \tag{1}$$

and arrive at the energy equation for multicomponent systems consisting of m different species:

$$\frac{\partial}{\partial t}\left(P + \sum_{i=1}^{m} C_i H_i\right) = -\nabla \cdot \left(q^{(x)} - k\nabla T + \sum_{i=1}^{m} N_i H_i\right) + v\nabla \cdot P + \tau : \nabla v + \sum_{i=1}^{m} j_i \cdot g_i \tag{2}$$

where ρ is the density, U is the internal energy per unit mass, v is the flow velocity, q is the heat flux, τ is the shear stress, g the acceleration of gravity, P and T are the thermodynamic pressure and absolute temperature respectively. C_i , j_i and N_i are the molar concentration, mass and molar fluxes of species i respectively, and k is the thermal conductivity.

Viscous Dissipation as a function of Aspect ratio for various Knudsen numbers (Kn)
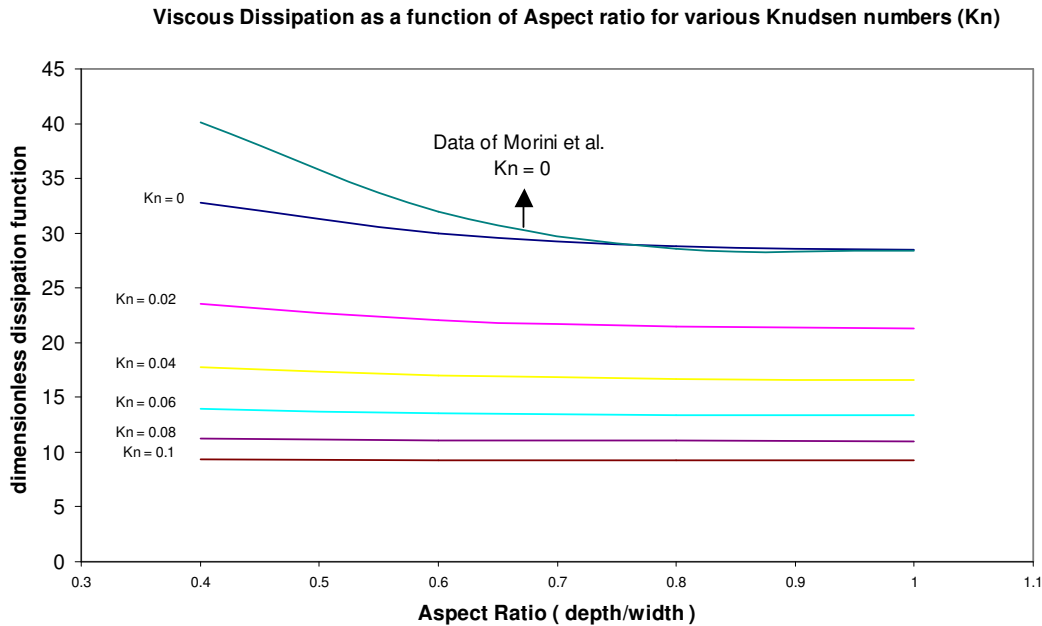

Figure 1 Effects of Knudsen number (Kn) on the dimensionless viscous dissipation. Upper curve shows data from [Morini et al. 1998], other curves are the results from our work.

In this work, the energy equation applicable to microfluidic flows in microchannels will be derived from the classical energy equation in its rigorous form. The significance of mass diffusion on the overall heat transfer rate in the absence of temperature gradients (Dufour effect) and the importance of other terms like viscous dissipation shown in Figure 1, which appear in the general form of the energy equation, will be addressed. In our work we propose a general formulation for $q^{(x)}$ in multicomponent systems in terms of $D_i^{(T)}$, the Dufour coefficient of species i, and new sets of dimensionless numbers that will aid in its

evaluation. This formulation reduces to the widely used Dufour expression for binary systems, and highlights the significance of this effect for microchemical applications. The final form of the energy equation that incorporates temperature jumps on the walls of the microchannel will be solved under some simplifying assumptions.

Our future study will address the problem of coupled mass and heat fluxes, and will detail a methodology for the evaluation of the temperature and concentration gradients in multicomponent microchemical systems. Due to this coupling, the effect of temperature difference on mass fluxes when there are no concentration gradients (Soret effect) will be included. A systematic approach for the evaluation of the concentration and temperature gradients in dilute systems will be illustrated as a special case.

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