

A Numerically Stable Method for Integration of the Multicomponent Species Diffusion Equations

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A diagonally implicit method is shown to be an effective method for integrating the multicomponent species conservation equations. The constitutive equation for multicomponent diffusion is recast into a form analogous to that for binary diffusion, except that the diffusion coefficient is replaced with a matrix of effective multicomponent diffusion coefficients. The resulting matrix has properties that allow the diagonal terms to be integrated implicitly and the off-diagonal terms to be integrated explicitly. Numerical experiments show the integration procedure is stable for time steps much larger than the diffusion equation time step condition.

Key Words: mass transfer, multicomponent diffusion, numerical stability