

A hybrid finite difference scheme for convection-diffusion problems in chemical engineering

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Abstract

Out of the different classes of methods suitable to solving boundary value problems defined by a set of partial differential equations, the finite differences method is easy to be implemented and can be an alternative to solve several classes of problems usually found in chemical engineering applications. One of the most commonly used discretization scheme is the central finite differences, which is second order accurate. However, despite its apparent simplicity, the method fails to converge when the problem under study is mostly dominated by convection [1].

In order to solve this issue, Griebel et al. (1998) [2] suggested implementing a hybrid scheme considering a weighted average of the central finite differences and the upwind difference scheme, the latter being a backward or forward discretization depending solely on the flux direction. Nevertheless, the author also cites that by following this procedure, the order of approximation will go from a second to a first order accuracy. Moreover, the classical upwind scheme suffers from numerical diffusion for systems defined by high values of Peclet numbers, which also compromises the accuracy of the numerical solution, providing a smooth solution to a highly stiff problem [1].

From this perspective, the present study is an attempt of following the suggestion of Griebel et al. (1998), by implementing the weighted average of both discretization schemes, modifying, however, the upwind method to a second order accurate backward/forward discretization scheme for the convective term. The weight employed is a function of the Peclet number calculated for the system. The approach has been tested against different 1D and 2D problems usually found in chemical engineering studies. The results obtained showed not only that the method is stable even for small number of discretization points and can obtain solutions with a high level of accuracy when compared to the real results for problems with analytical solutions.

Keywords

Finite Differences, Convection-Diffusion, Mathematical Modeling

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References

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