

327f Numerical Problem Solving in Undergraduate Reaction Engineering

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Experience in using a user-friendly software, Mathcad, in the undergraduate chemical reaction engineering course is discussed. Example problems considered for illustration deal with simultaneous solution of linear algebraic equations (kinetic parameter estimation), nonlinear algebraic equations (equilibrium calculations for multiple reactions and steady state behavior of isothermal/non-isothermal CSTR with single/multiple reactions), integral equations (design of steady-state plug flow reactor, PFR), integral-algebraic equations, and nonlinear ordinary differential equations (solution of conservation equations for steady-state PFR and unsteady state CSTR). The capabilities of Mathcad are of significant benefit in accelerating the learning and strengthening the fundamental knowledge base.