## ABSTRACT

Modeling of reactors, fixed, fluidized or moving beds, is usually a very complex exercise. It involves chemical reaction, heat and mass transfer with varying contacting patterns. Single-particle reaction features assume great importance in this exercise. Often, in detailed reactor modeling, a simplified single-particle reaction model is used. However, it limits the applicability of the model. The present investigations are directed towards bridging this gap and incorporating detailed single particle reaction model in overall reactor analysis.

Gas-Solid Non-Catalytic (GSNC) reactions have immense industrial applications. Due to their diverse nature, GSNC reactions can not be generally explained by one single model. Detailed analysis of these reactions have been carried out based on Shrinking Core/Sphere and Volume Reaction Models. Finite Volume Method, not yet applied for general analysis of GSNC reactions, has been employed for solution. The present model predictions have been found to agree well with the analytical solution, numerical and experimental results of other workers reported in the literature. Detailed parametric studies have been carried out to assess the effects of different model parameters on the progress of reaction. The geometric and thermal instabilities have/investigated in detail.

Combustion and pyrolysis reactions are two important examples of such reactions. Combustion reactions for carbon, lignite and coal char have been modeled using Shrinking Core/Sphere and Volume Reaction Models, incorporating both the heterogeneous and homogeneous reactions. Ignition/extinction phenomena have been investigated. The effect of various process variables on the the combustion dynamics has been studied in detail. A two-stage kinetic-heat transfer model is developed for the pyrolysis of biomass and experiments carried out to verify the model. The model is found to explain the pyrolysis behaviour of large and small biomass particles adequately. Parametric studies have also been carried out. Combustion data on high ash Indian coal in fluidized bed is still limited. Some useful experimental design data have been generated for combustion of high ash Indian coal and biomass in a batch Fluidized Bed Combustor (FBC) fabricated for the purpose. Single-particle combustion of high ash Indian coal and electrode carbon is carried out in FBC and the mass-loss and temperature profiles are used to validate the combustion models developed. Finally the detailed single-particle reaction model has been incorporated in overall reactor analysis of Fluidized Bed Combustor for the combustion of coal char.

## **KEYWORDS:**

Modeling and Simulation, Combustion, Coal Char, Pyrolysis, Biomass, Gas-Solid Non-Catalytic (GSNC) Reactions, Sharp Interface Model (SIM), Shrinking Core Model (SCM), Shrinking Sphere model (SSM), Volume Reaction Models (VRM), Moving Boundary Problem, Numerical Solution, Finite Volume Method (FVM), Thiele Modulus, Biot Number, Effectiveness Factor, Conversion, Burn-out Time, Ignition, Extinction, Fluidized Bed Combustor (FBC), Population Balance, Twophase Theory.