# Applications of the Constrained Gibbs Energy Method in Modelling Thermal Biomass Conversion

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## ABSTRACT

Constrained Gibbs free energy method (CFE) is applied for modelling super-equilibrium concentrations in biomass gasification and formation of NO emissions during biomass combustion.

Super-equilibrium refers here to the state of chemical system where excess amounts of certain species as compared with global equilibrium at given temperature and pressure are observed. For example the formation of methane, tar, ammonia and char in biomass gasification and biomass and over-shoot of free radicals and related NO emissions may then be contemplated using the super-equilibrium hypothesis.

Super-equilibrium concentrations for the NO emissions are derived from the mechanistic reaction rate models. When biomass gasification is considered the observed relations based on the experimental results are utilised as conditional constraints. Results confirm that constrained Gibbs energy method is a feasible practice for modelling these thermal biomass conversion processes.

CFE method can be seen as a good alternative for conventional approaches in several modelling applications where coupled kinetics and thermodynamics are needed.