Group contribution modelling for the prediction of safety-related and environmental properties - DTU Orbit (08/11/2017)

Group contribution modelling for the prediction of safety-related and environmental properties

We present a new set of property prediction models based on group contributions to predict major safety-related and environmental properties for organic compounds. The predicted list of properties includes lower and upper flammability limits, heat of combustion, auto ignition temperature, global warming potential and ozone depletion potential.

Process safety studies and environmental assessments rely on accurate property data. Safety data such as flammability limits, heat of combustion or auto ignition temperature play an important role in quantifying the risk of fire and explosions among others. Global warming potential and ozone depletion potential became a standard to analyze the environmental impact of processes and products.
In the early stage of process development and analysis, experimental values are often not available due to cost or time constraints. In this case property prediction models like group contribution (GC) models can estimate data. However, the estimation needs to be accurate, reliable and as little time-consuming as possible so that the models can be used on the fly.

In this study the Marrero and Gani group contribution (MR GC) method has been used to develop the models for safety-related and environmental properties. The method considers the group contribution in three levels: The contributions from a specific functional group (1st order parameters), from poly-functional (2nd order parameters) as well as from structural groups (3rd order parameters). The latter two classes of GC factors provide additional structural information beside the functional group. The contributions of all three factors are then summed up. For the database, DIPPR are used together with the reported measurement accuracy. For parameter estimation, a comprehensive statistical methodology was followed to improve prediction accuracy and reliability (95% confidence).

The method is simple and easy to apply. Taking into account higher order groups increases the accuracy. Furthermore, the application range is high due to the high number of considered functional and structural contributions.

A thorough uncertainty analysis provides information about the prediction error, which is important for communicating the reliability of the predicted values for the user for potential applications in process safety studies and environmental assessments.

Example application of the models are shown for a selected class of chemicals to highlight the application range of models.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Frutiger, J. (Intern), Abildskov, J. (Intern), Sin, G. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from AIChE 2016 Spring Meeting and 12th Global Congress on Process Safety, Houston, United States.
Main Research Area: Technical/natural sciences
Electronic versions:

AIChE_Spring_2016_GC_Method_Jerome_SUBMITTED.docx
Source: PublicationPreSubmission
Source-ID: 122777666
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016