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Data-driven modelling of a pelleting process and prediction of pellet physical properties

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In the production of pelleted catalysts products, it is critically important to control the physical properties of the pellets, such as their shape, density, porosity and hardness. Maintaining these critical quality attributes (CQAs) within their in-specification boundaries requires the manufacturing process to be robust to process disturbances and to have good knowledge of the relationships between process parameters and product CQAs. This work focuses specifically on increasing understanding of the impact of pelleting process parameters on pellet CQAs, and the development of data-driven models to predict and thereby monitor product CQAs, based on information from the pelleting machine instruments. A Compaction Simulator machine was used to produce over 1000 pellets, whose properties were measured, using varied feeder mechanisms and feed rates. Exploratory analysis was used to summarise the key differences between experimental conditions, and partial least squares and support vector regression was used to predict pellet density from the Compaction Simulator data. Pellet density was predicted accurately, achieving a coefficient of determination of 0.87 in 10-fold cross-validation, and 0.86 in an independent hold-out test. Pellet hardness was found to be more difficult to predict accurately using regression, therefore, we opted to use a support vector classification approach to classify pellets as 'in-spec'or 'out-of-spec'. In testing, the resultant classification model correctly classified 100% of the out-of-spec pellets (recall) and 90% of the pellets classified as out-of-spec were correctly classified (recall). Overall, the modelling process provided insights into process parameter-CQA relationships and demonstrated the possibility to monitor pellet quality using sensor data without the need for random sampling and destructive testing of pellets.

Keywords

Multivariate analysis, machine learning, pelleting process monitoring

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