466g Modelling and Design of Non-Ideally Mixed Batch and Semi-Batch Reactor Systems

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Batch reactor systems are increasingly important for the production of fine chemical and pharmaceuticals. In such reactors the interplay between mixing, reaction and mass transfer (for multi-phase reactors) significantly affects the system's performance. In this work we investigate macro-mixing effects in batch and semi-batch reactors by constructing 3-dimensional models using a network of zones (NoZ) discretisation. System dynamics including volume changes due to continuous feeding are successfully predicted. Detailed flow fields are calculated from phenomenological correlations which include parameters such as reactor size and configuration, impeller type and speed and fluid physical properties. Flow fields are then superimposed on the computed dynamic mass balances using a multi-grid discretisation scheme. The Proper Orthogonal Decomposition method is subsequently applied to extract reduced models from the large-scale NoZ-based ones that can be used for computationally efficient design, optimisation and optimal control studies.

Furthermore, we are presenting a model based on population balances and on the pivot method which we have extended to account for all the important phenomena taking place in these systems such as droplet breakage and coalescence, mass transfer between phases and reactions. We are combining this model with our Network of Zones model to efficiently simulate non-ideally mixed liquid-liquid systems.

We use illustrative case studies for the literature to validate our models and to demonstrate our design and optimisation methodologies.