Synthesis of Nanoparticles in Continuous Microreactors: a Link between Residence Time Distribution and Particle Characteristics

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Highlights

- The residence time distribution effect on continuous nanoparticle synthesis was studied.
- A model for predicting the particle size distribution was developed.
- Good agreement between model and experiments was observed.

1. Introduction

Nanomaterial synthesis is a research topic of increasing interest in many areas such as electronics, energy, biotechnology and medicine. Large scale production of nanoparticles is commonly based on batch reactors. However, product properties obtained from different batches can be irreproducible. Furthermore, quality screening procedures are difficult to implement in this type of reactors, and scaling up is a challenge (due to the difficulties in achieving uniform concentration and temperature conditions at the timescale required).

For these reasons, continuous-flow systems are gaining increasing attention as a tool for nanoparticle synthesis. Milli- and micro-reactors can be employed to synthesise nanoparticles in a continuous process, ensuring high productivity and enhanced controllability of the process, as well as easy implementation of on-line control devices [1]. To adopt these reactors in industrial applications, efficient design procedures must be developed. This requires the understanding of the spatio-temporal evolution of the reactions and transport phenomena taking place in the reactor during the synthesis. We present here a predictive model based on residence time distributions, attempting to provide an insight in some of the relevant transport phenomena that affect reactor performance. We tested the model using the synthesis of silica nanoparticles via the Stöber process as a case study. Two different reactor configurations were modelled: a single-phase laminar flow reactor (LFR) and a two-phase segmented flow reactor (SFR). The results were validated against data from the literature [2].

2. Methods

The kinetics of the Stöber process was first modelled using a population balance approach according to the aggregative model proposed by Bogush and Zukoski [3], using batch data from the literature [2]. The kinetic parameters obtained were subsequently used to model the continuous reactors (LFR and SFR). These reactors were modelled through different residence time distributions, depending on their characteristic flow conditions.

The LFR was described according to the approach proposed by Ananthakrishnan et al [4], taking into account the difference in diffusivity between the different components of the reaction mixture. The SFR was modelled as an ideal plug flow reactor. The particle size distribution obtained in the continuous flow reactors was determined by an averaging procedure over the residence time distributions of the reactors.

3. Results and discussion

Figure 1 shows the comparison between the model results and the data from the literature for both LFR and SFR, in terms of average size of the particle size distribution (PSD) and its relative standard deviation (i.e. normalized over the average size). The model predicted the trend observed experimentally in a satisfactory way. Taking into account the residence time distributions, the model was able to predict the behavior of the continuous reactors (LFR and SFR) starting from data obtained in batch experiments. Comparing the two types of reactors, the SFR led to larger and more monodisperse particles, at the cost of a more complex reactor operation [2].

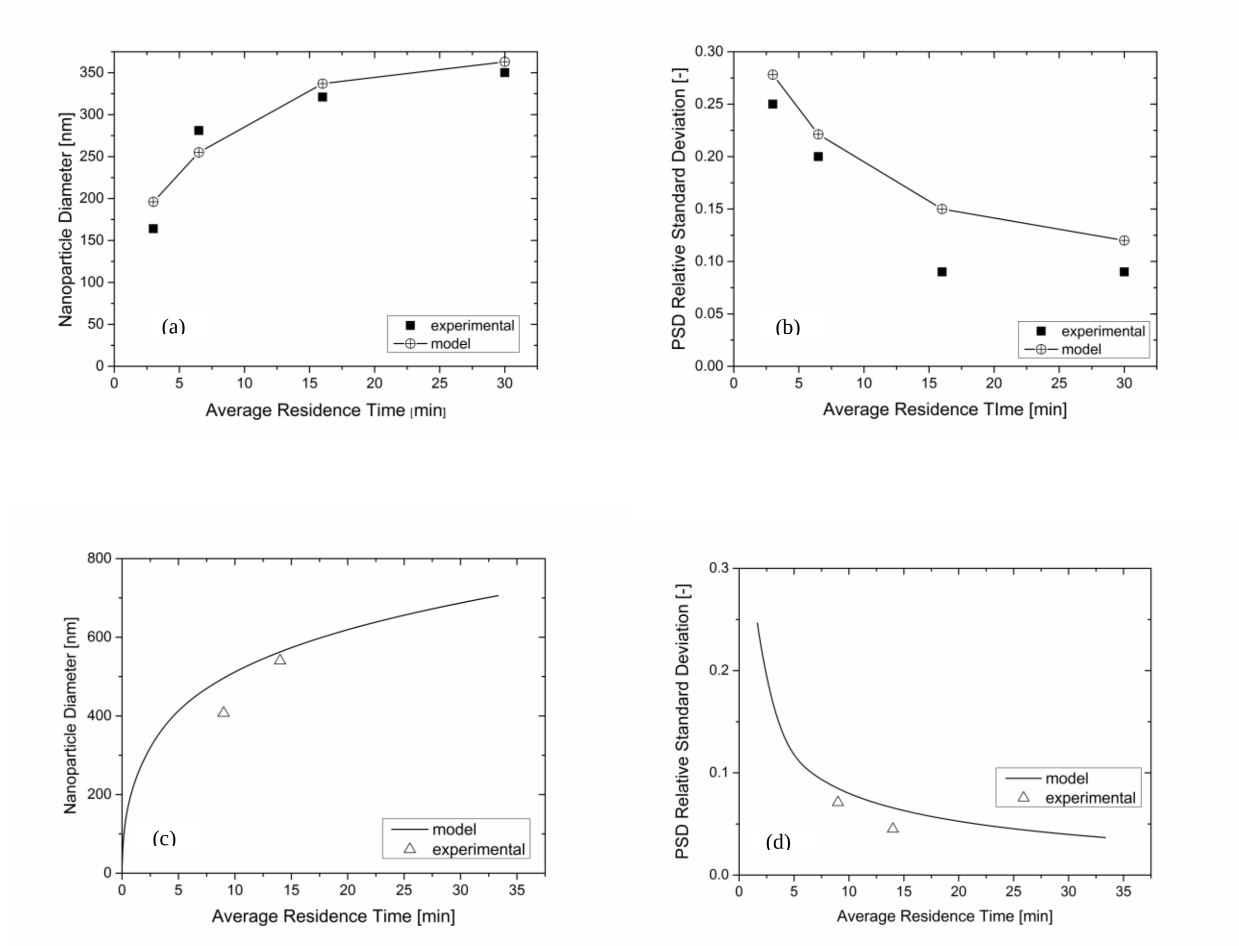

Figure 1. Comparison between model results and experimental data for different residence times τ: Average particle size (a) and relative standard deviation of PSD (b) obtained in the LFR. Average particle size (c) and relative standard deviation of PSD (d) obtained in the SFR.

4. Conclusions

A model for the continuous synthesis of nanoparticles in continuous flow microreactors was developed and applied to a case study. The use of residence time distributions and kinetics obtained by fitting literature batch experimental data led to the satisfactory prediction of the output of a laminar flow and a segmented flow reactors, without the need of any adjustable parameters. The model aims to contribute towards a more refined design procedure of continuous flow reactors for synthesising nanoparticles of desired characteristics.

References

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“Microreactor”, “Nanoparticles”, “Reactor Design”, “Laminar Flow Reactor”