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REVIEW OF DOCTORAL THESIS

Intensyfikacja przereagowania cieplnie sprzężonych układów reaktorów chemicznych pracujących w systemie rewersyjnym"

(Intensification of conversion in systems of thermally-coupled chemical reactors operated in reverse flow)

Submitted by Bożena Kulik to the Faculty of Chemistry
Silesian University of Technology, Gliwice, Poland

1 Subject of the thesis and its significance

The thesis is essentially a theoretical and numerical study, and deals with the innovative configuration and operation of systems of chemical reactors, with the purpose of intensification of the yield. Particularly, the analysis first concentrates on a single non-adiabatic cascade of CSTR in reverse-flow and then on more complex systems, namely two thermally–coupled, independently reversible cascades of CSTR arranged in co–current flow as well as counter–current flow. The systems are equipped with an external jacket. The aim of the study is basically a brute–force optimization aimed at intensifying the conversion in the system by determining the best configuration among various variants. Since the systems considered are periodically forced, most regimes are non–stationary: hence, the notion of average conversion degree is introduced and employed.

The problems considered in the thesis are undoubtedly important from a practical point of view. The tackled differential problems are not too complex in their mathematical formulation and numerical implementation, however the configurations and combinations examined lead to complex dynamical behavior, also because of the discontinuity in the boundary conditions due to flow–reversal. This makes them difficult to study in terms of bifurcation analysis, as conventional continuation algorithms cannot be successfully used. Indeed, the approach via the Poincaré section of the dynamical system, adopted in this study, overcomes the discontinuity difficulty.

In conclusion, topic and instruments used in the thesis can be judged as well selected.

2. Abilities shown by the candidate

The candidate has conceived and modeled a complicate chemical engineering problem in view of innovating/improving the relevant process. She has demonstrated a good understanding of physical background of the constituent problem and appears to have a good command of the numerical methods employed. She has diligently reported on the results obtained during her research work.

The literature cited in the dissertation (74 items) is properly selected, although one or two issues should perhaps have been covered more extensively and accurately, as explained below.

In conclusion, the dissertation shows that Ms Kulik has the ability to deal with conceptually complex problems, by successfully formulating and solving relevant engineering and scientific tasks, after proper recollection and evaluation of the relevant scientific background, and conclusively report in a clear and organized way the result of her study.

3. Scientific value of the work

The thesis work in fact moves from the model reported in [1] (why Reference [1], co-authored by Ms Kulik, is not listed? See Critical remarks below) and extends much further with the analysis of several different configurations, to the aim of intensifying the generic process conducted in the system. The configurations identified constitute a substantial improvement in terms of process intensification, with respect to what is obtainable by standard means. Remarkable and unconventional is the idea of exploiting dynamical regimes to achieve higher conversion.

In order to make the dissertation suitable for publication in a journal, a selection must be made of the abundant figures and cases reported, and additional cases should be considered, for example by coupling exothermic and endothermic processes in the two thermally coupled cascades (see Critical remarks below).

In conclusion, the work has significant scientific value.

4. Style and readability

The thesis contains a clear description of the background, correctly indicates the scope and effectively report the conclusions. The account of the simulations for the many selected cases could have used a better arrangement: the way it is, a rather flat sequence of figures and captions, is more adapt to a technical report.

In conclusion, the thesis is sufficiently readable in that the information can be easily recovered, but the style does not excite my enthusiasm.

5. Critical remarks

5.1 I do not understand why the thesis does not make reference to a paper co-authored by the candidate and published in 2008 [1], as the paper is relevant to the subject of the thesis. This publication by the way testifies the scientific value of the subject.

5.2 The use of thermally coupled reactors has long been proposed and studied, even with reverse flow [2, 3] although, as the candidate states in the thesis, the particular configuration chosen (thermally coupled cascade of CSTR) is not found in the literature. As seen in Refs [2, 3], thermal coupling is best suited to gain efficiency by coupling two distinct chemical processes – one exothermic and the other endothermic. The dimensionless model presented by the candidate allows for different sets of values of the parameters between the two streams, but the cases explored are all relevant to the same reaction in both cascades. Why?

5.3 The literature cited should have included References 2 and 3, as they relate to topics which are strictly connected to the subject of the thesis.

5.4 The analysis, including assessment of conversion improvement, is always referred to an average value of conversion. This is obvious, because the regimes considered are dynamical. However, it is

not obvious how the average conversion is calculated. Is it an integral average? If yes, how is the integration domain chosen?

5.5 The work opens up a world of possible further developments, however there is no mention or comment regarding future work.

Minor:

5.6 The remark after Fig. 5.3 is obvious but presented as if it were unexpected.

5.7 A Table reporting the improvement in the conversion for the various cases would be very helpful in summarizing the results.

6. Evaluation of the work

Ms Bożena Kulik has shown the ability of conceiving and modeling complicate chemical engineering problems in view of innovating/improving the relevant process. Particularly, both configuration and operation modes were investigated by integrating innovative up-to-date solutions. Particularly, a remarkable result consists of the improvement of conversion by resorting to dynamic regimes. Conclusions are drawn that do not relate to a specific chemical process, on the contrary they are of general interest. The contribution has remarkable scientific value and should be considered for publication after revision.

In view of this, the thesis meets all requirements of a doctoral dissertation. It is my pleasure to recommend to the Board of the Faculty of Chemistry of the Silesian University of Technology the dissertation entitled:

"Intensyfikacja przereagowania cieplnie sprzężonych układów reaktorów chemicznych pracujących w systemie rewersyjnym"
(Intensification of conversion in systems of thermally-coupled chemical reactors operated in reverse flow)

by Ms Bożena Kulik

as suitable for further processing within the procedure of conferring the doctoral degree.

Gaetano Continillo
Professor

References

[1] B. Kulik and M. Berezowski, Chaotic dynamics of coupled cascades of tank reactors with flow reversal. *Chemical and Process Engineering* 29 (2008) 465–471

[2] M. van Sint Annaland, H. A. R. Scholts, J. A. M. Kuipers,W. P. M. van Swaaij, A novel reverse flow reactor coupling endothermic and exothermic reactions. Part I: comparison of reactor configurations for irreversible endothermic reactions. *Chemical Engineering Science* 57 (2002) 833–854

[3] M. van Sint Annaland, H. A. R. Scholts, J. A. M. Kuipers,W. P. M. van Swaaij, A novel reverse flow reactor coupling endothermic and exothermic reactions. Part II: Sequential reactor configuration for reversible endothermic reactions. *Chemical Engineering Science* 57 (2002) 855–872