



# Software Enhanced Research iN Transient kinetics

## Rapports

### Informations projet

#### SERENiTi

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Projet clôturé

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UNIVERSITEIT GENT



Belgium

## Periodic Reporting for period 1 - SERENiTi (Software Enhanced Research iN Transient kinetics)

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### Résumé du contexte et des objectifs généraux du projet



An existing user-friendly software, that had been commercialized already for steady-state simulation purposes, has found new application areas by the incorporation of the possibility to account for important transient phenomena. The latter are commonly encountered in industry as startup, shutdown and perturbations of the continuous flow reactor operation. Moreover, the implementation of a transient solution strategy has rendered the software more robust, even for steady-state simulations. Yet, the transient features come at the expense of an increased computational cost and, hence, a

judicious balance should be made between solution methodology and the benefits brought about by this methodology. Regarding the reaction kinetics determination, implementing the possibility of transient kinetic data analysis has provided to possibility to acquire more insight into the underlying reaction mechanism. On the catalyst surface scale, catalyst deactivation as an inevitable transient phenomenon can now be explained and solved in terms of microkinetics, i.e. elementary reaction steps. The software has been promoted and gained significant interest at specialized conferences in the field on the national, European and global level. A workshop has been organized which has been able to attract 30 attendees from all over Europe with about & third coming from industry.

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