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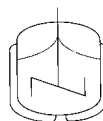
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## Modelling

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## Overcoming performance and convergence issues of discrete transform based modeling of crosslinking classical and reversible deactivated radical polymerizations

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Population balances of polymer species in terms of discrete transforms with respect to counts of groups lead to tractable first order partial differential equations when all rate constants are independent of chain length and loop formation is negligible [1]. Average molecular weights in the absence of gelation are long known to be readily found through integration of an initial value problem. The extension to size distribution prediction is also feasible, but its performance is often lower to the one provided by methods based upon real chain length domain [2]. Moreover, the absence of a good starting procedure and a higher numerical sensitivity has decisively impaired its application to non-linear reversibly deactivated polymerizations, namely NMRP [3]. Here, a new kind of Picard iteration applied to the two point boundary value problems (2PBVP) arising from the solution of population balance by the method of characteristics was introduced. It can lead to initial estimates for standard numerical methods for 2PBVP or as a standalone procedure. CPU time is about 20 times lower than for case studies in [2]. The annoying usability and convergence problems previously found when tackling non-linear NMRP also belong to the past, as shown by the successful calculation of gel fraction and sol average molecular weight shown in Figures 1 and 2. Compared to predictions shown in Fig. 2, experimental results in [4] show a general qualitative agreement, with a delayed gel time (at conversion 0.5 rather than 0.3), which is not unexpected since loop formation reactions have been neglected in these calculations.

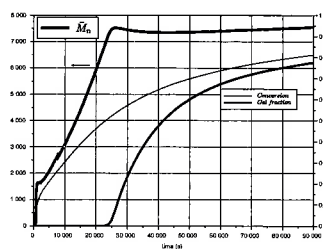


Fig. 1: 84 mmol/L BPO + 100 mmol/L TEMPO at the start

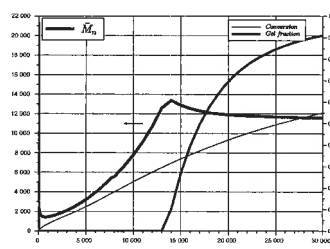


Fig. 2: 34 mmol/L TEMPO adduct at the start

Predicted monomer conversion, gel weight fraction and sol  $M_n$  vs. time for batch bulk styrene + 1.6% mol 4,4'-divinylbiphenyl at 125 °C

### References:

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