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Supporting Information for "Jacket temperature regulation allowing well-defined non-adiabatic lab-scale solution free radical polymerization of acrylates"

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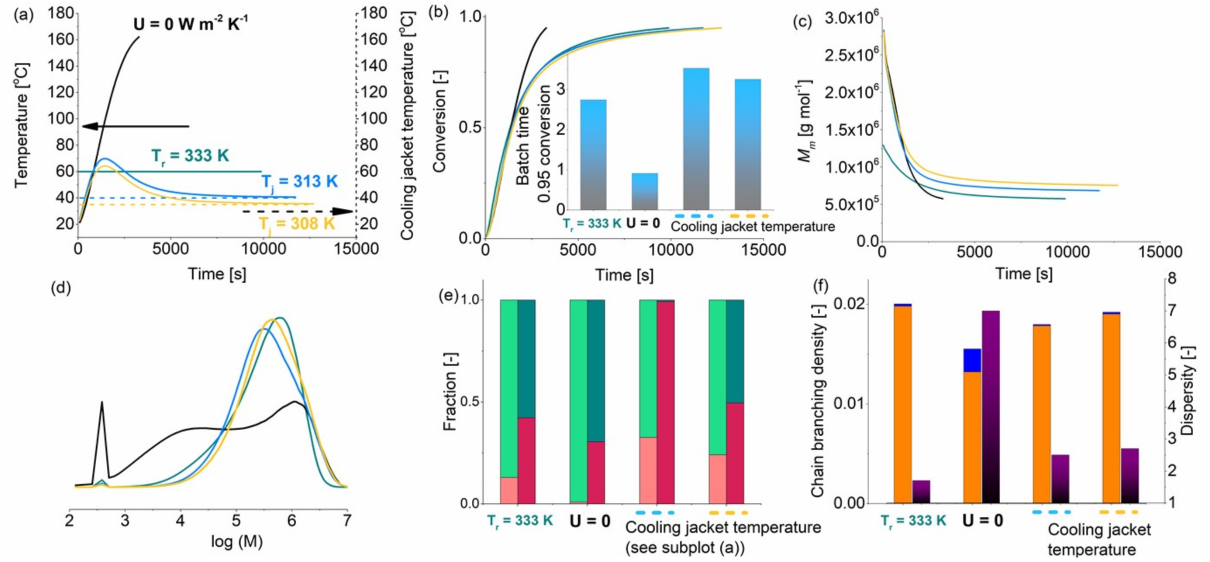

Figure S1. Comparing adiabatic and non-adiabatic reactor operations for solution free radical polymerization (FRP) of *n*-butyl acrylate (*n*BuA) with $[n\text{BuA}]_0 = 3.3$ mol L^{-1} and and $T_{r,0} = 298$ K but applying the zeroth order initiation case with AIBN. Evolution of (a) reactor temperature (left axis) and jacket temperature (T_{jacket}; right) axis as a function of time, (b) monomer conversion as a function of time as well the final batch time for 0.9 (monomer) conversion, (c) mass average molar mass M_m as a function of time and (d) molar mass distribution (MMD) (w(log *M*) format) at a monomer conversion of 0.90; (e) fractions of macromonomer and dead polymer at a monomer conversion of 0.90 with light- green/red number fraction and dark-green/red: mass fraction, (f) left axis: orange and blue: short and long chain branching density at a monomer conversion of 0.90, (f) right axis in dark-purple dispersity at 0.90 monomer conversion; blue: $T_{\text{jacket}} = 313$ K, yellow: $T_{\text{jacket}} = 308$ K, black: adiabatic operation with *U* in Equation (1) equal to 0 instead of 100 W m^{-2} K^{-1}(the dimension of *U* is omitted in the figure), dark-cyan: isothermal (theoretical) at 313 K; Arrhenius parameter in Table 1.

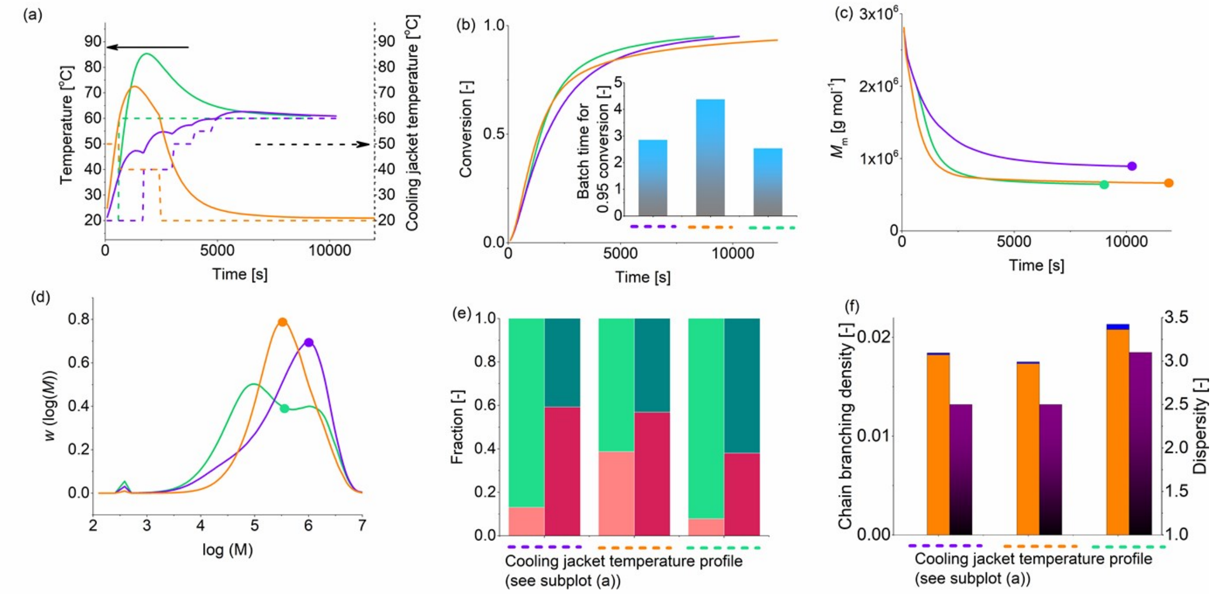

Figure S2. Same outline as in Supplementary Figure S1 considering three non-adiabatic cases with stepwise jacket temperature (T_{jacket}) control; orange: $T_{\text{jacket}} = 323$, 313, 293 K, green: $T_{\text{jacket}} = 293$, 333 K, violet $T_{\text{jacket}} = 293$, 313, 323, 328, 333 K.

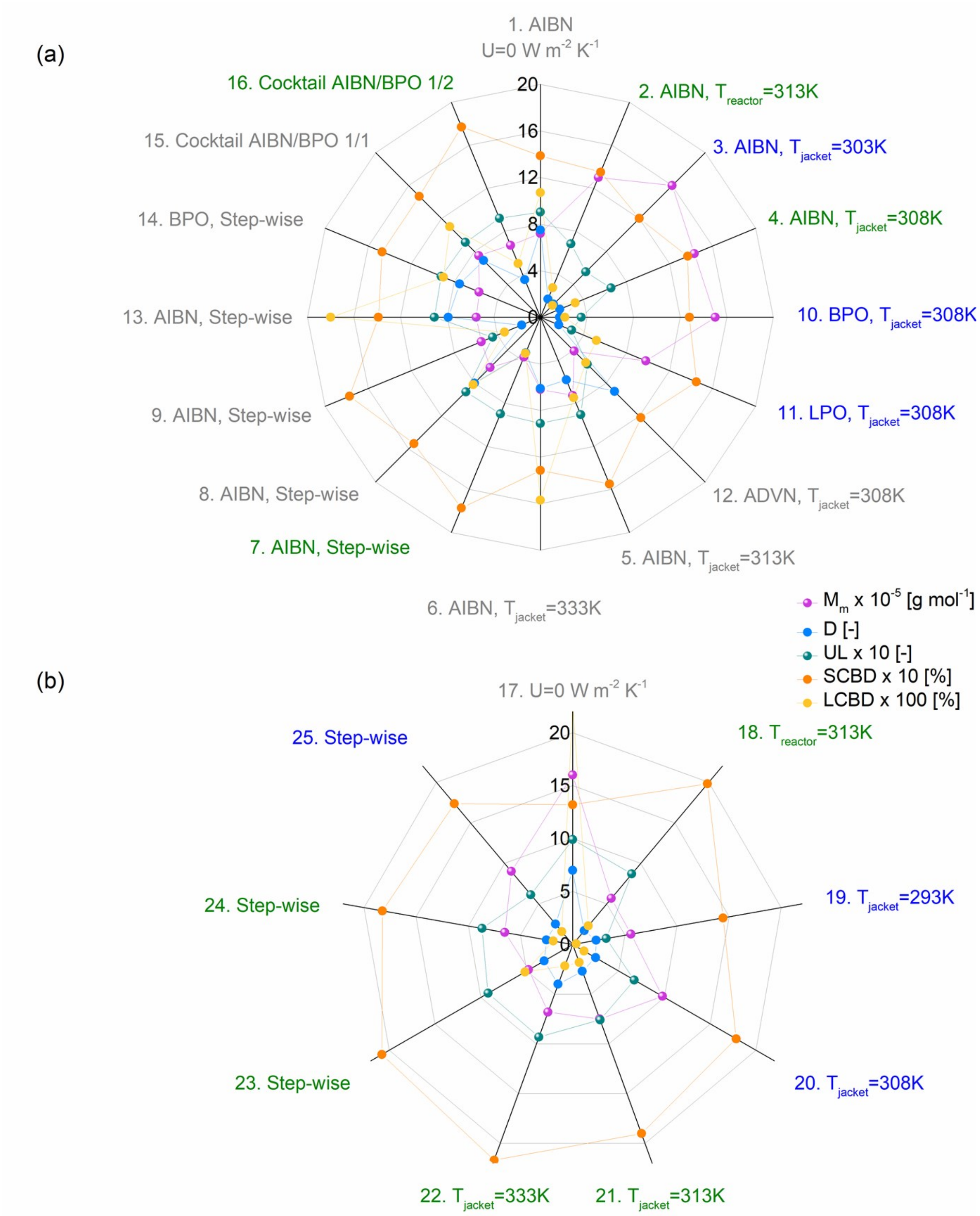

Figure S3. Radar charts with absolute data (normalized in Figuee 11).

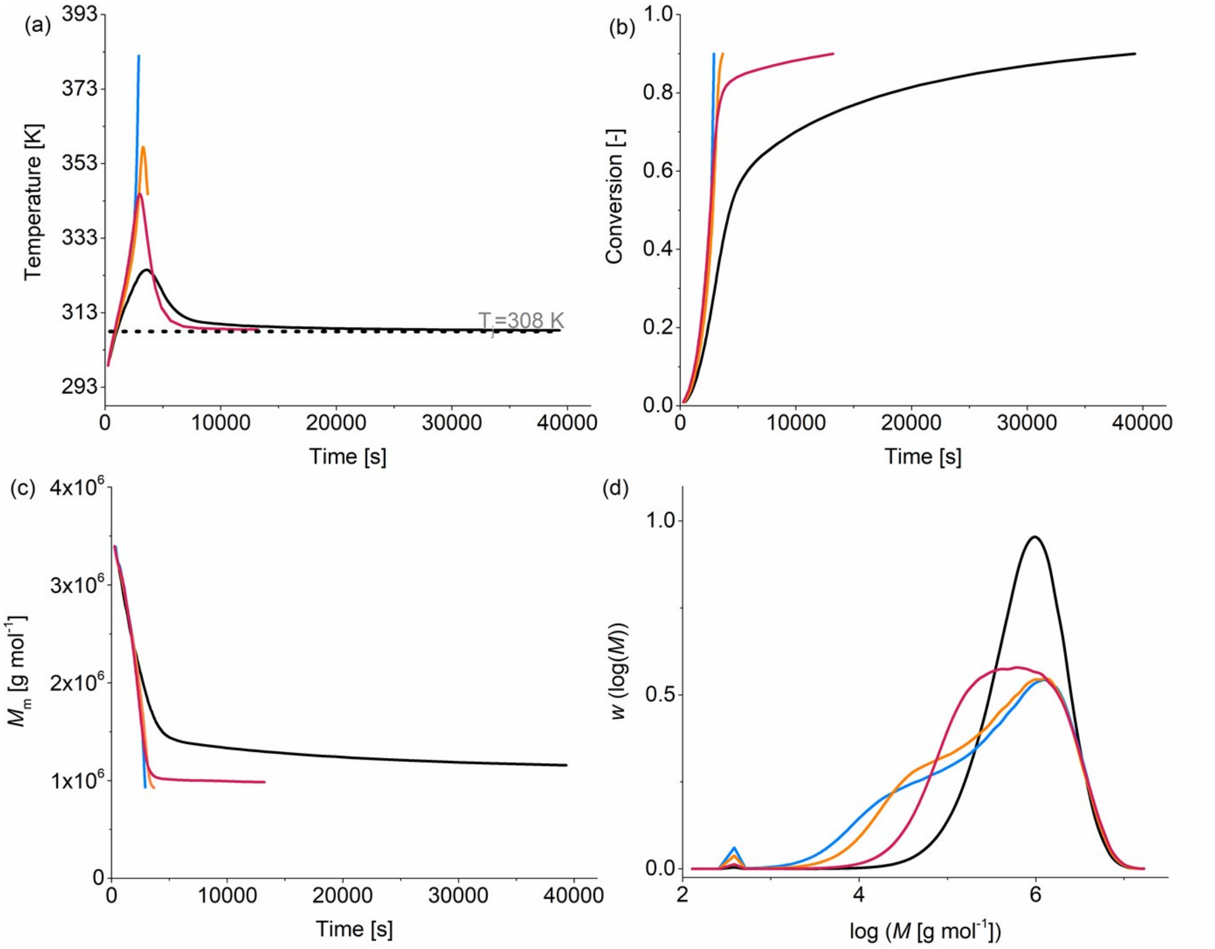

Figure S4: Influence of under/overestimated activation energies for backbiting and β-scission (while also varying pre-exponential factors) on the predicted: (a) reactor temperature, (b) monomer conversion, (c) mass average molar mass M_m as a function of time, and (d) log-molar mass distribution (MMD) at 0.9 monomer conversion; flat jacket temperature T_{jacket} = 308 K. All rate coefficients equal to the reference values listed in Table 1, except for: orange: $E_a^{backbiting}$ = 34.7 kJ mol^{-1}, $A^{backbiting}$ = 1.6× 10^8 s^{-1} provided by Barth *et al.*[1] blue: $E_a^{backbiting}$ = 31.7 kJ mol^{-1}, $A^{backbiting}$ = 4.48× 10^7 s^{-1} provided by Nikitin *et al.*[2], dark-red: $E_a^{backbiting}$ = 55.0 kJ mol^{-1}, $A^{backbiting}$ = 2.8× 10^{11} s^{-1} provided theoretically by Cuccato *et al.*[3]; black: reference values; $[M]_0$ = 3.3 mol L^{-1}; $[AIBN]_0$ = 3×10^{-3} mol L^{-1} and $T_{r,0}$ = 298 K; U = 100 W m^{-2} K^{-1}.

References:

1. J. Barth, M. Buback, P. Hesse and T. Sergeeva, *Macromolecules*, 2010, **43**, 4023-4031.
2. A. N. Nikitin, R. A. Hutchinson, M. Buback and P. Hesse, *Macromolecules*, 2007, **40**, 8631-8641.
3. D. Cuccato, E. Mavroudakis, M. Dossi and D. Moscatelli, *Macromolecular Theory and Simulations*, 2013, **22**, 127-135.