Table S1. Comparison of Performance of Common Simplification Schemes for Different Reaction Networks

	Method	Applicable system	Initial mechanism source	Calculation of kinetic parameters	Computational cost	Chemical interpretability	Speedups
Skeleton simplification	DRG, DRGEP[1]	Hydrocarbon combustion, large-scale oxidation networks (10^3–10^4	Detailed mechanism	Retain original rate	Low	√	~100
	PFA[2]	High-carbon fuel pyrolysis/oxidation, cyclic reaction networks	Detailed mechanism	Retain original rate	Low	√	~100
Reduction based on time scale	QSSA[3]	Gas-phase chain reactions, combustion, small-molecule pyrolysis	Skeleton mechanism	Rate constants unchanged	Middle	×	~100
	CSP[4]	Multi-time-scale systems (combustion, catalysis, atmospheric chemistry)	Detailed/skeleton mechanism	Rate constants unchanged	High	√	~100
Lump	Lump[5]	Polymer pyrolysis, heavy hydrocarbon cracking, petroleum refining	Experimental data	Fit lumped rate constants	Middle	×	(-)
	Reax-Lump (This work)	**Polymer pyrolysis**	**ReaxFF MD**	**Fit lumped rate constants**	**Middle**	**√**	**1000~10,000**
Data-driven method	CRNN[6]	Polymer pyrolysis, biological catalysis	Experimental data	Fit lumped rate constants	High	×	(-)
	SRG-Reax[7, 8]	Hydrocarbon fuel	Detailed mechanism	rate constants unchanged	High	√	~100

Note*: Speed-up refers to the reduction multiple of the kinetic mechanism

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