

Appendix A

See Figs. [A.1](#), [A.2](#), [A.3](#) and [A.4](#).

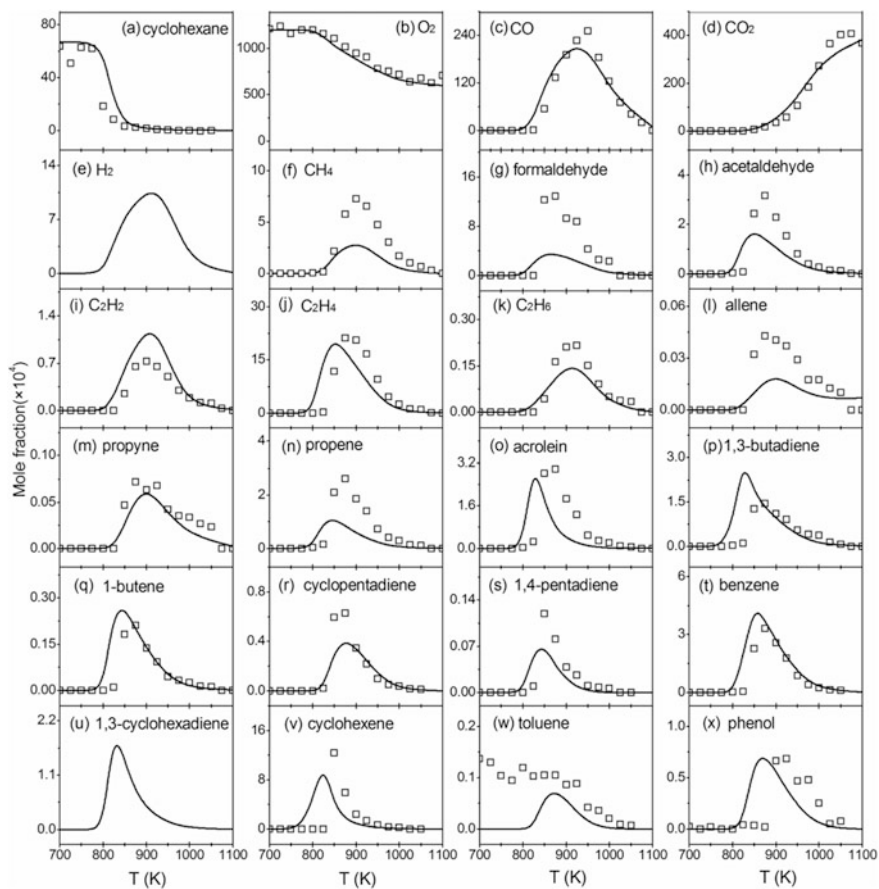


Fig. A.1 Experimental (symbols) and simulated (lines) mole fraction profiles of reactants, major products, and C1–C7 intermediates during cyclohexane oxidation with equivalence ratio of 0.5 and pressure of 1.05 atm

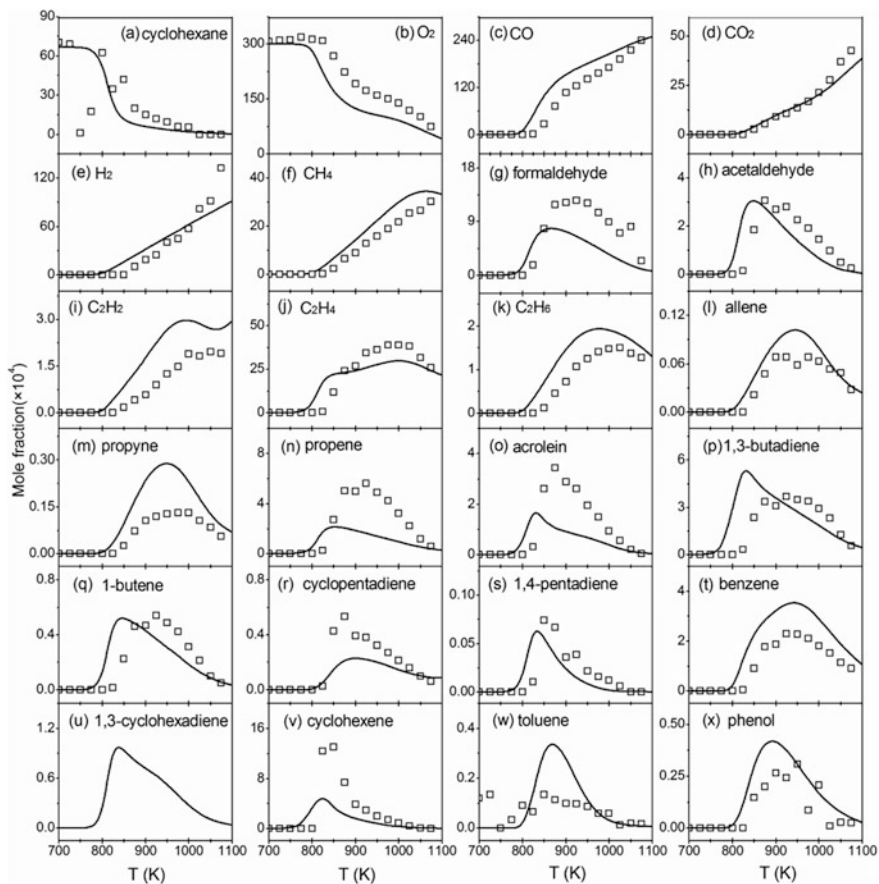


Fig. A.2 Experimental (symbols) and simulated (lines) mole fraction profiles of reactants, major products, and C1–C7 intermediates during cyclohexane oxidation with equivalence ratio of 2.0 and pressure of 1.05 atm

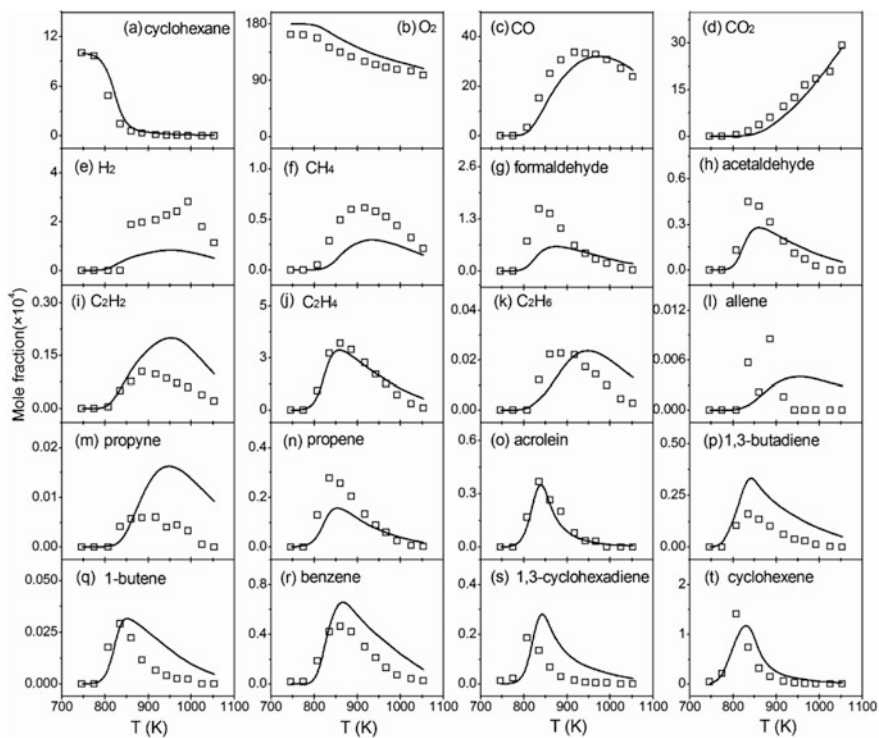


Fig. A.3 Experimental (symbols) and simulated (lines) mole fraction profiles of reactants, major products, and C1–C6 intermediates during cyclohexane oxidation with equivalence ratio of 0.5 and pressure of 10 atm

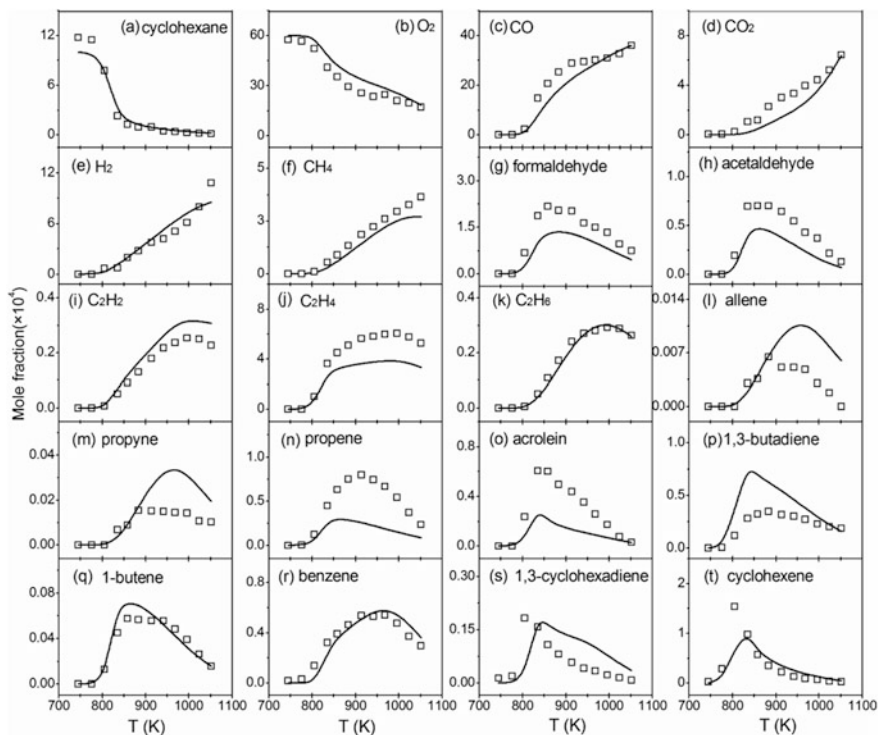


Fig. A.4 Experimental (symbols) and simulated (lines) mole fraction profiles of reactants, major products, and C1–C6 intermediates during cyclohexane oxidation with equivalence ratio of 1.5 and pressure of 10 atm

Appendix B

See Figs. B.1, B.2, B.3 and B.4.

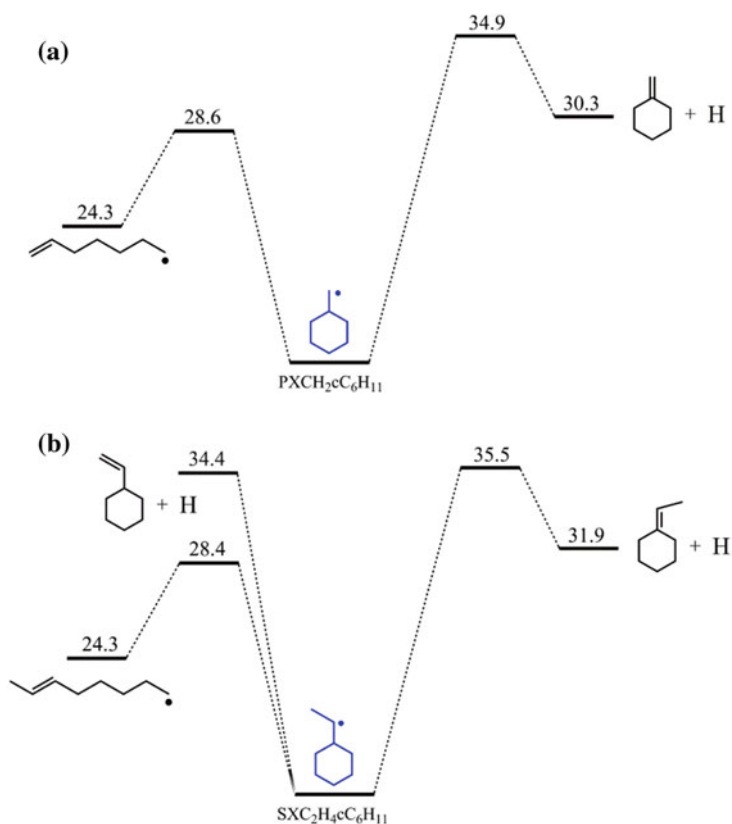


Fig. B.1 Potential energy surfaces for the unimolecular reactions of cyclohexylmethyl radical (a) and 1-cyclohexyl-1-ethyl radical (b). Reprinted from Ref. [18] in Chap. 5, Copyright 2015, with permission from Elsevier

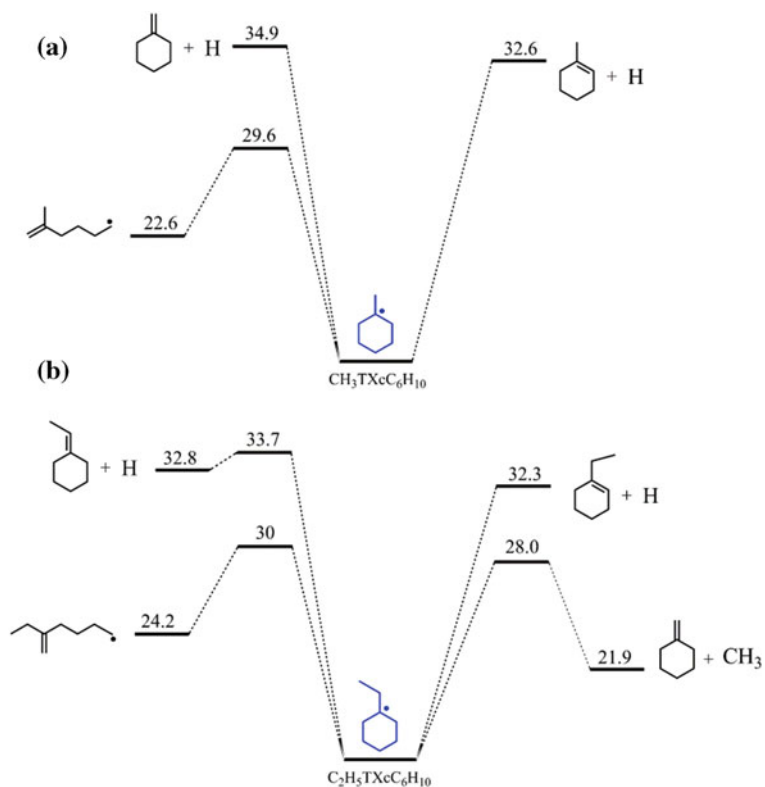


Fig. B.2 Potential energy surfaces for the unimolecular reactions of 1-methyl-cyclohexyl radical (a) and 1-ethyl-cyclohexyl radical (b). Reprinted from Ref. [18] in Chap. 5, Copyright 2015, with permission from Elsevier

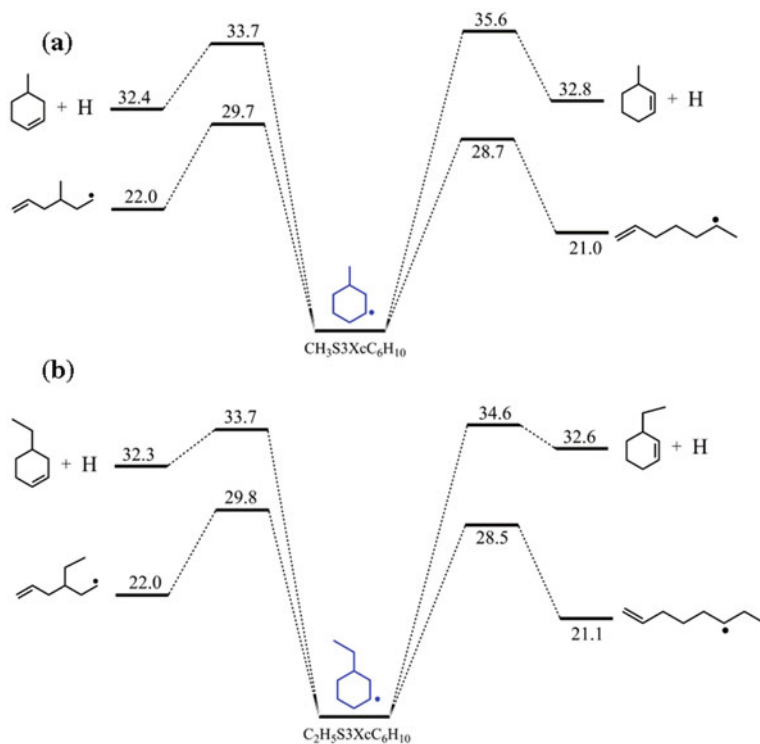


Fig. B.3 Potential energy surfaces for the unimolecular reactions of 3-methyl-cyclohexyl radical (a) and 3-ethyl-cyclohexyl radical (b). Reprinted from Ref. [18] in Chap. 5, Copyright 2015, with permission from Elsevier

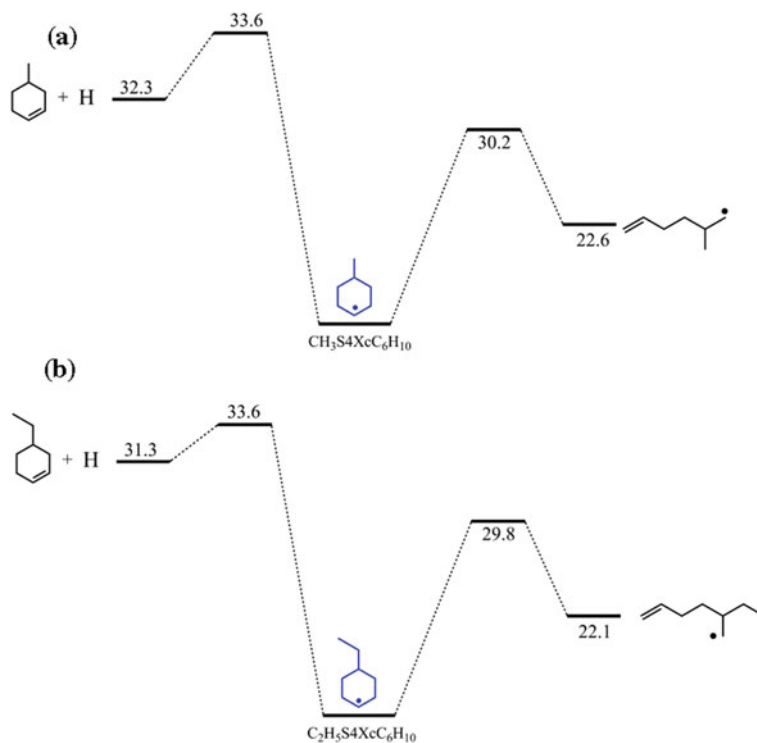


Fig. B.4 Potential energy surfaces for the unimolecular reactions of 4-methyl-cyclohexyl radical (a) and 4-ethyl-cyclohexyl radical (b). Reprinted from Ref. [18] in Chap. 5, Copyright 2015, with permission from Elsevier

Appendix C

See Figs. C.1 and C.2.

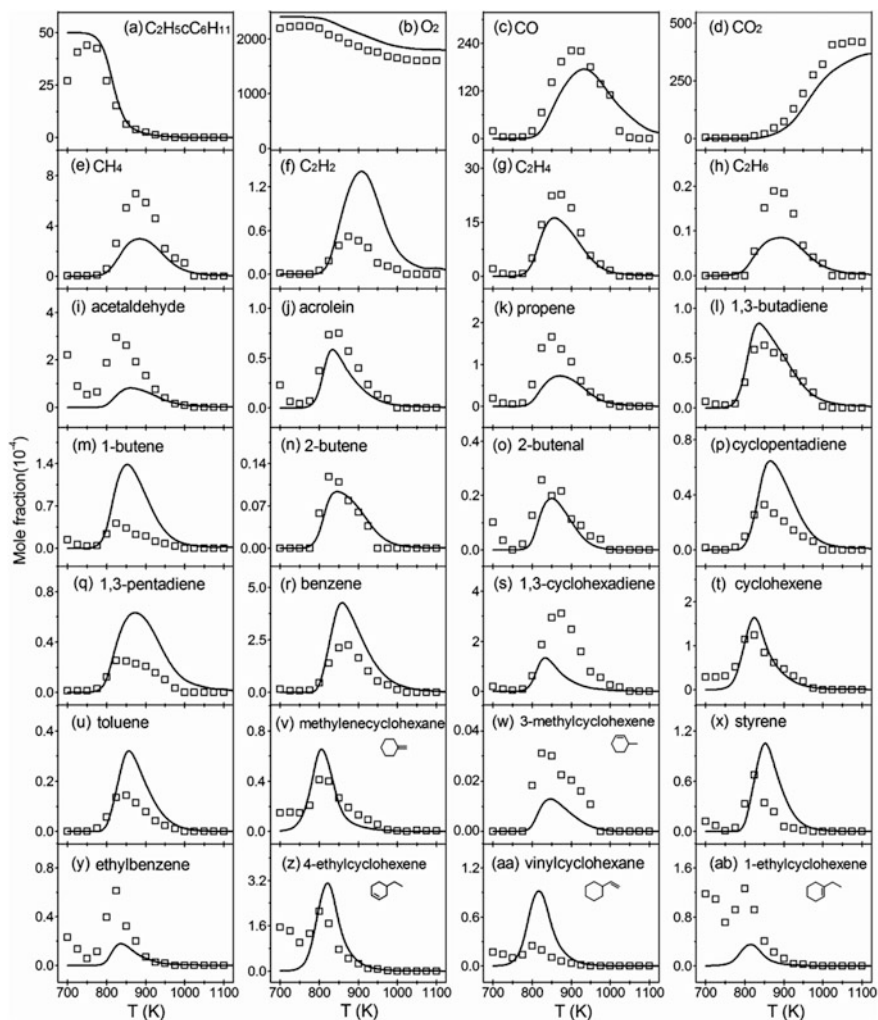


Fig. C.1 Mol fraction profiles of reactants, major oxidation products, and C1–C8 intermediates in ethylcyclohexane oxidation at 800 Torr and equivalence of 0.25. Symbols from literature data of Husson et al. Lines from simulation. Reprinted from Ref. [18] in Chap. 5, Copyright 2015, with permission from Elsevier

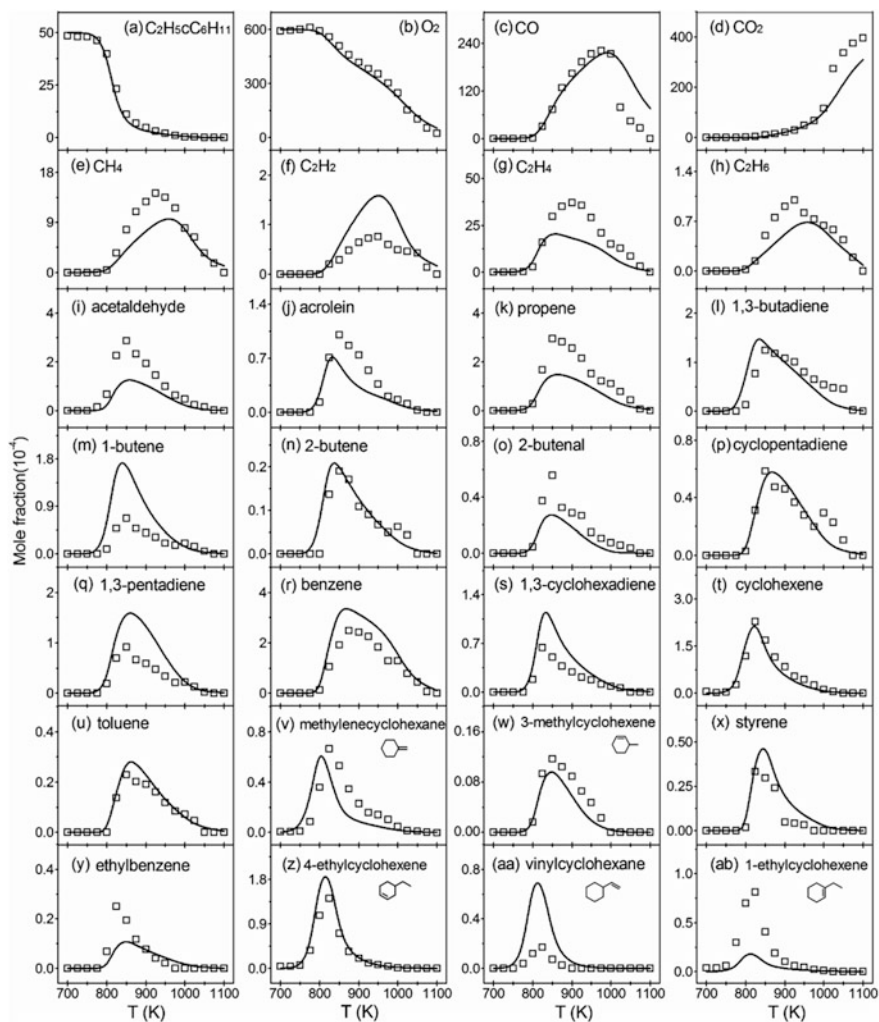


Fig. C.2 Mol fraction profiles of reactants, major oxidation products, and C1–C8 intermediates in ethylcyclohexane oxidation at 800 Torr and equivalence of 1.0. Symbols from literature data of Husson et al. Lines are from simulation. Reprinted from Ref. [18] in Chap. 5, Copyright 2015, with permission from Elsevier