

Hierarchical auto-ignition and structure-reactivity trends of C₂–C₄ 1-Alkenes

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Supplemental Information

1. Mechanism performance for ethylene

1.1 Shock tube ignition delay times of ethylene

1.1.1 Hidaka et al. experimental data[1]

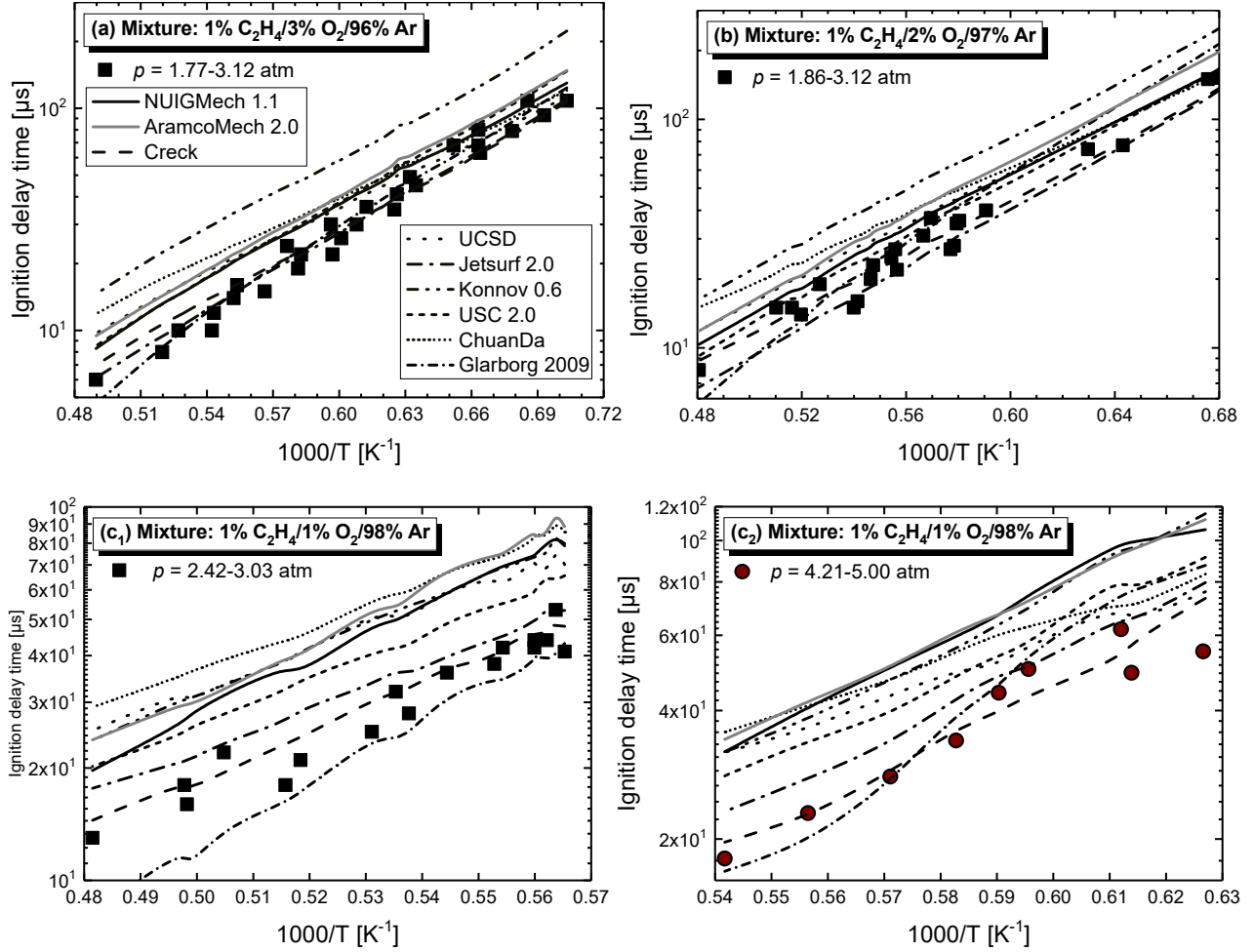


Figure S1: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.2 Brown and Thomas experimental data[2]

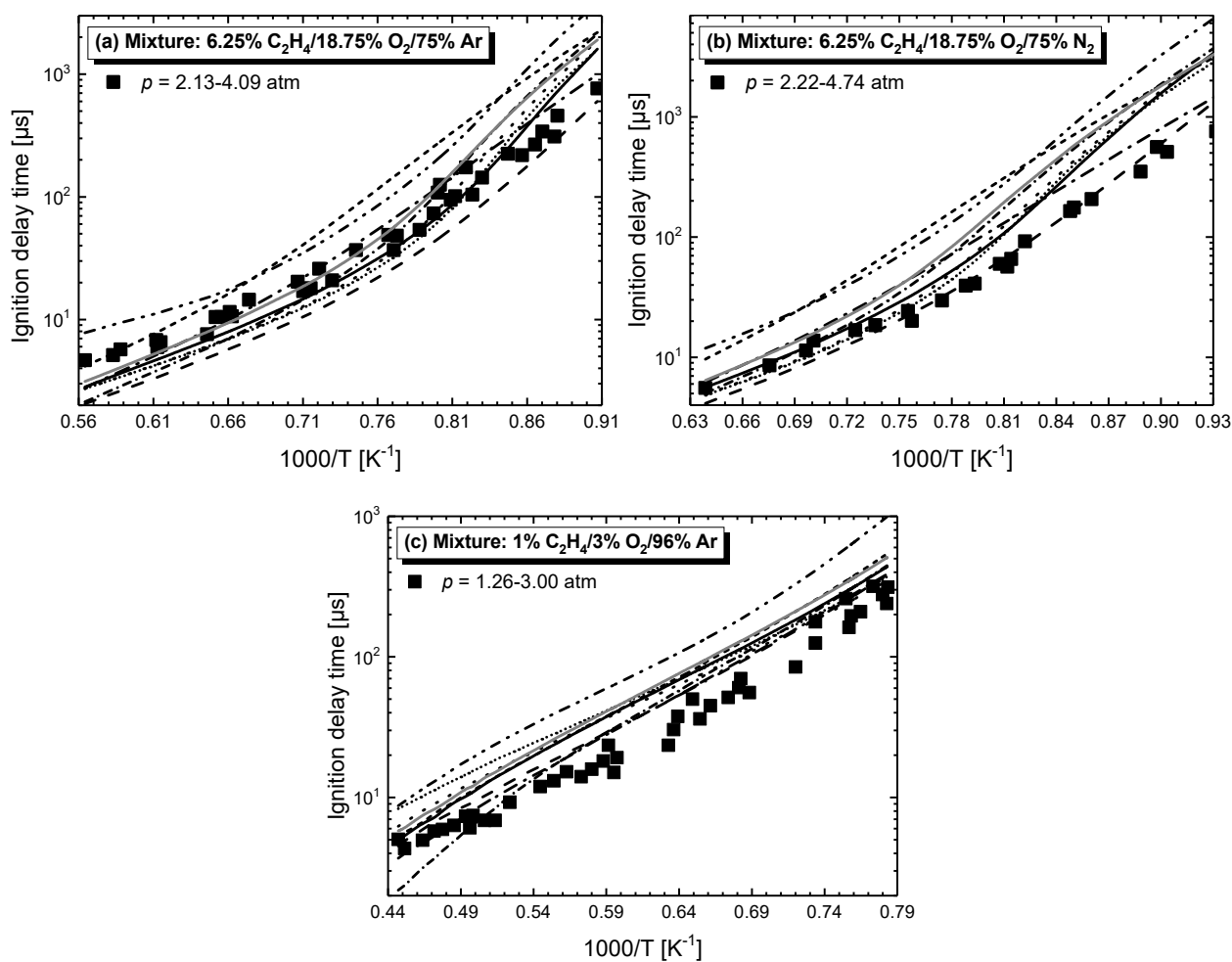


Figure S2: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.3 Collect and Spadaccini experimental data[3]

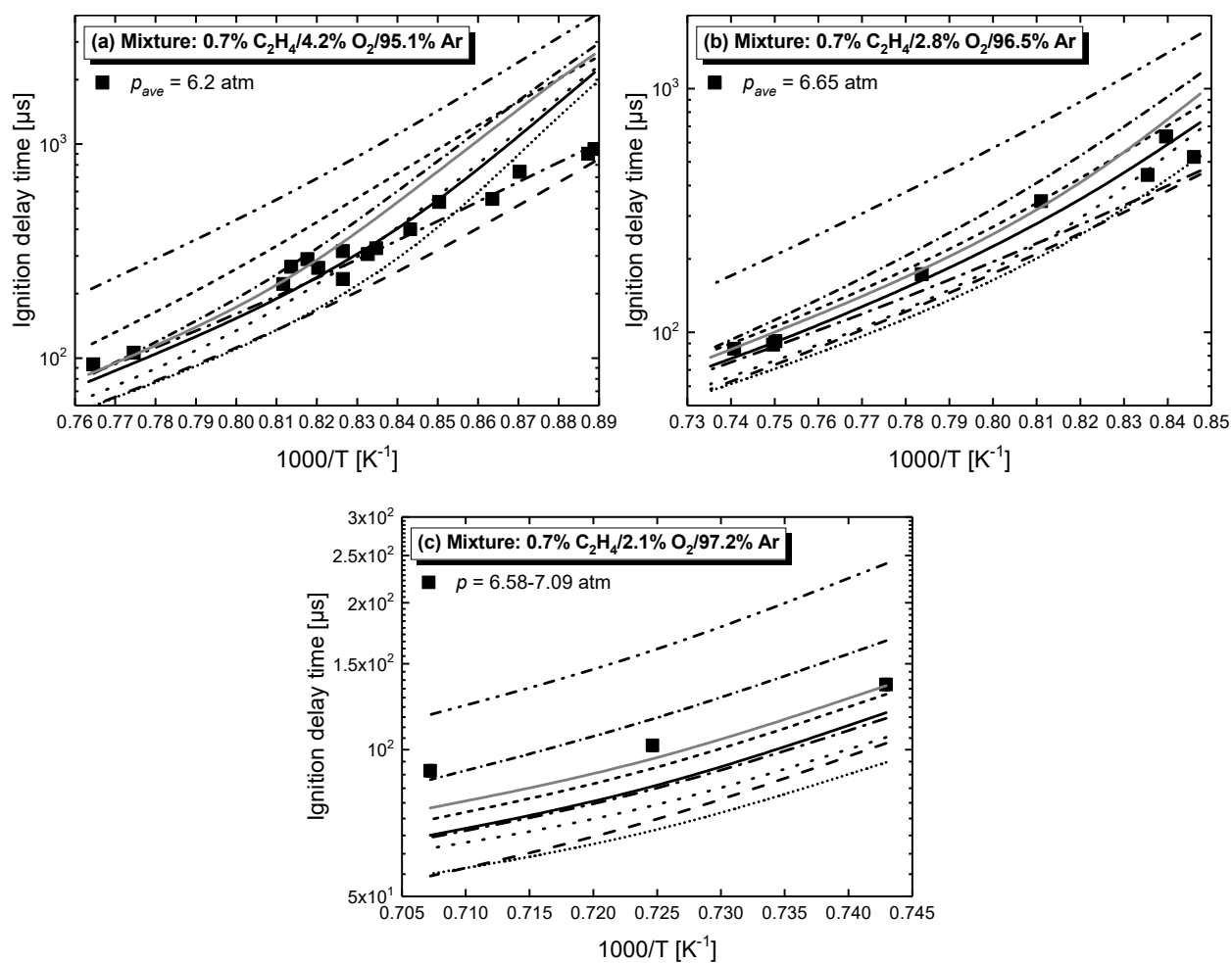


Figure S3: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.4 Horning experimental data (Stanford)[4]

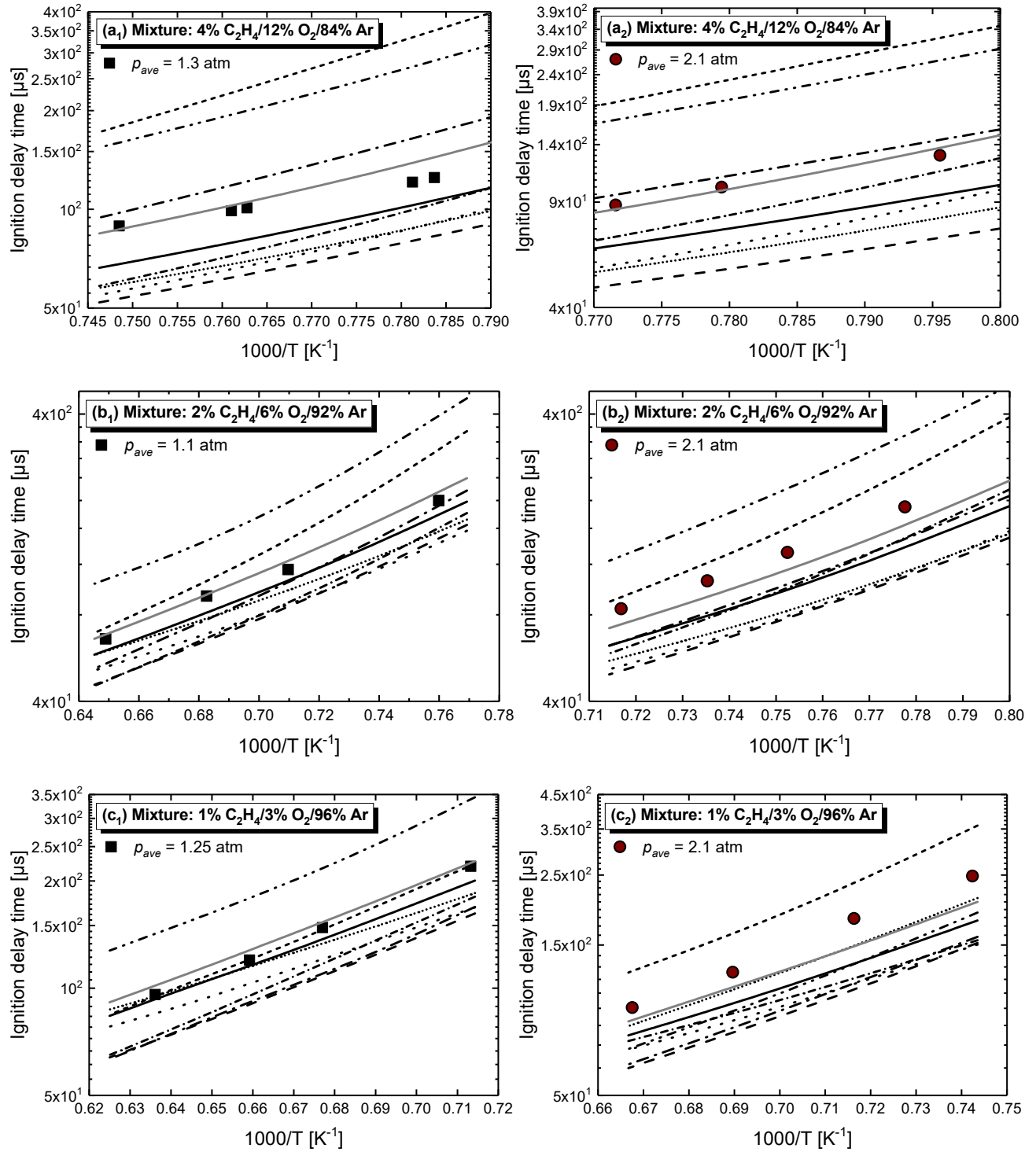


Figure S4: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.5 Kalitan et al. experimental data[5]

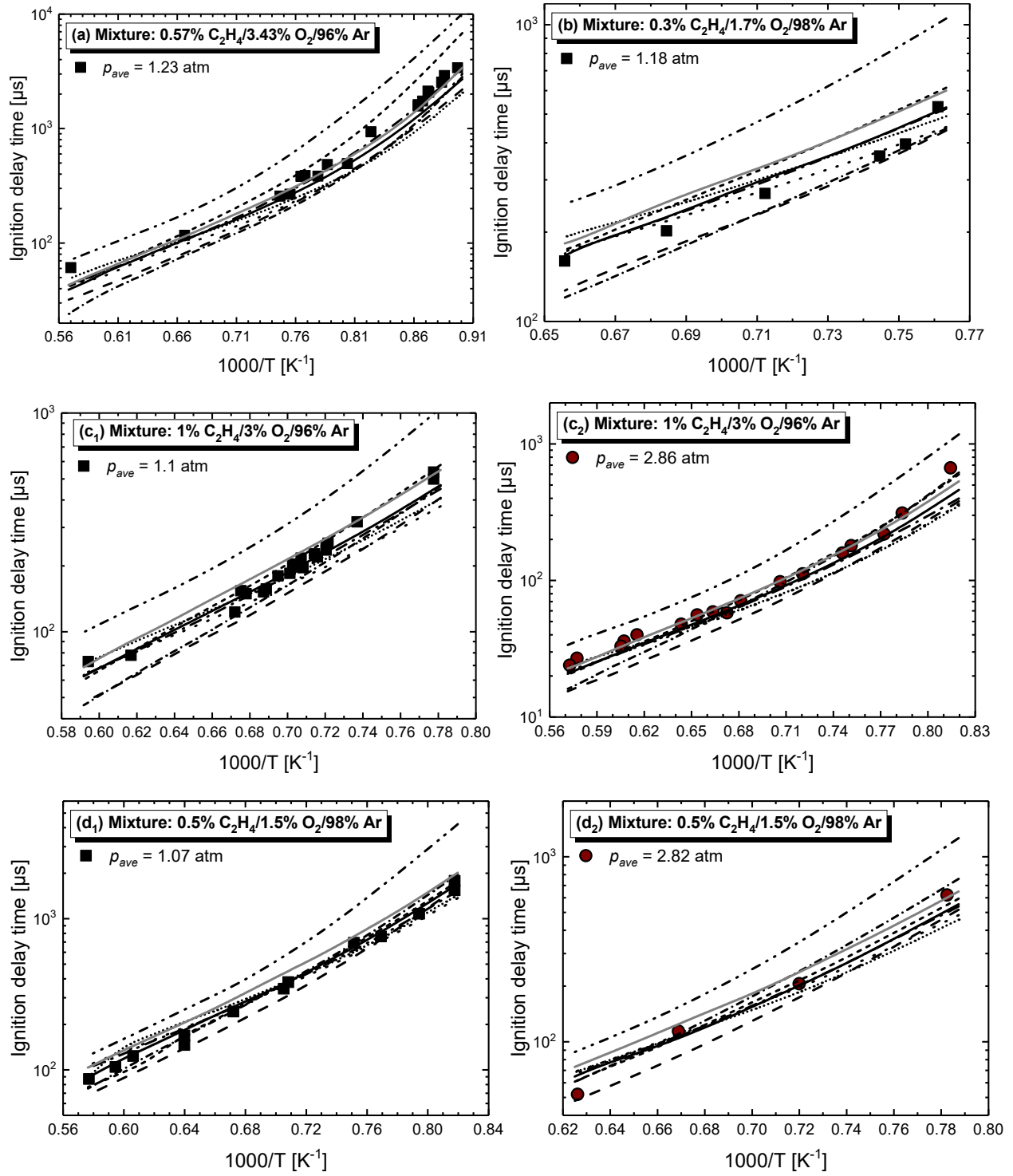


Figure S5: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.6 Penyazkov et al. experimental data[6]

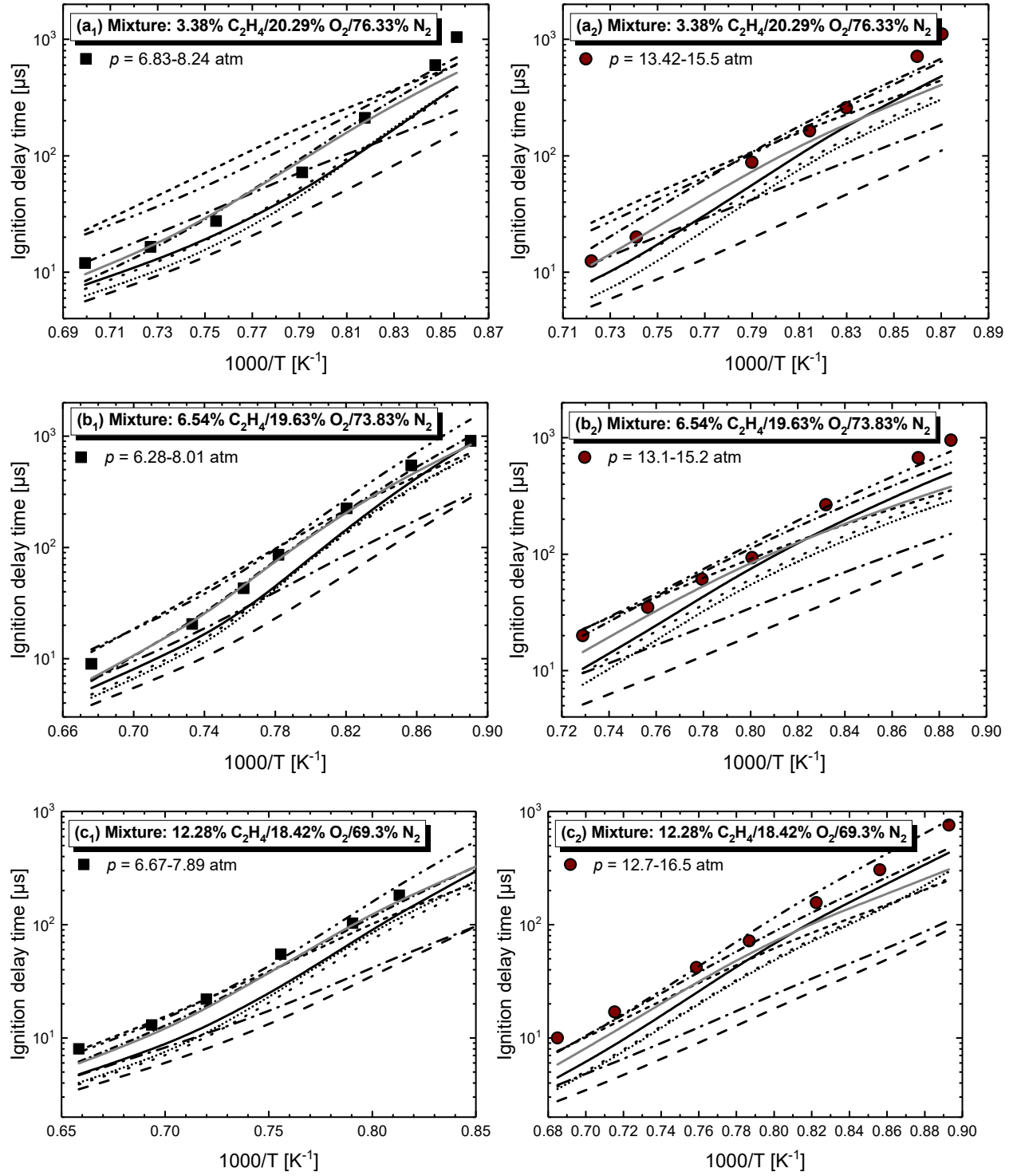


Figure S6: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.7 Tereza et al. experimental data[7]

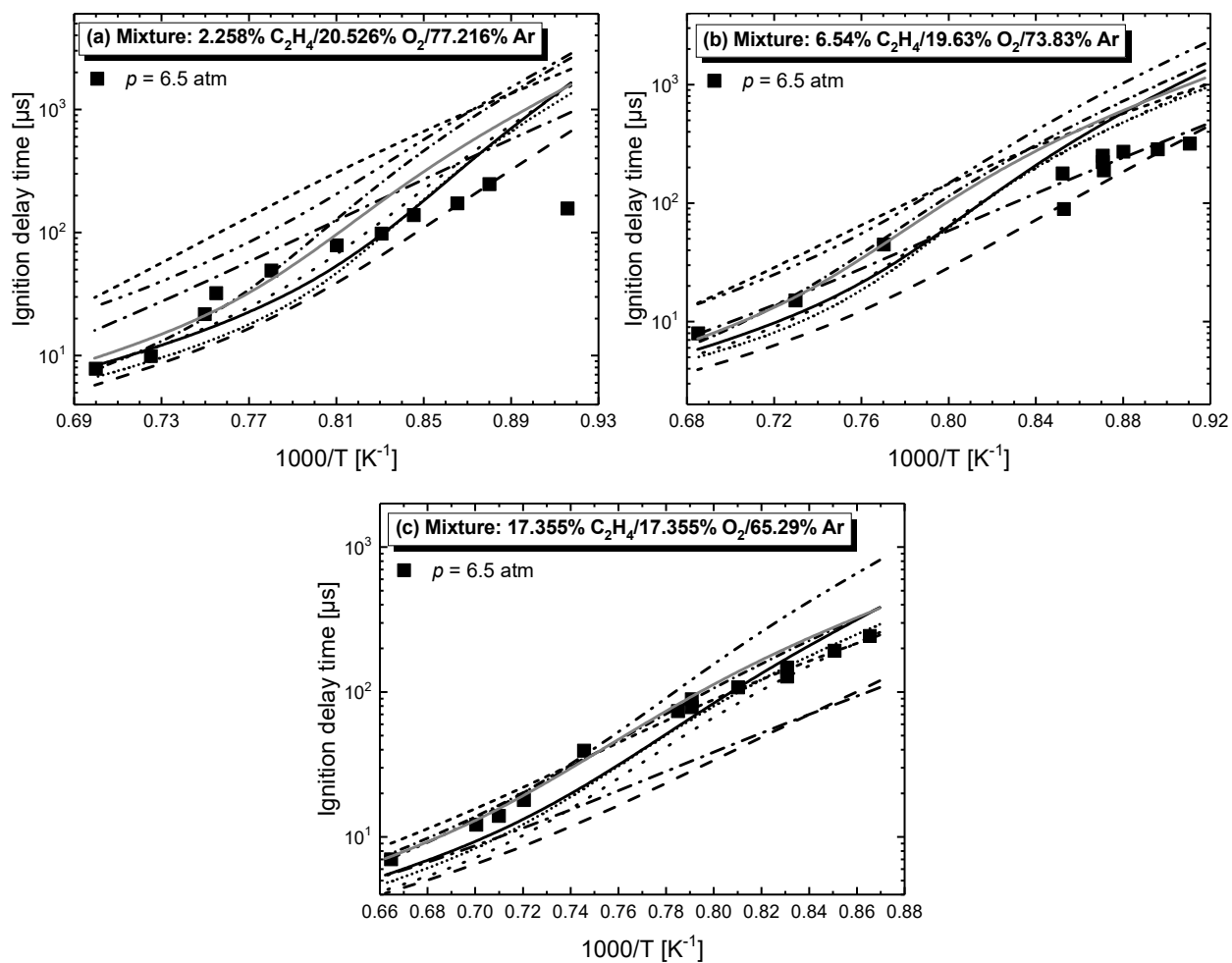
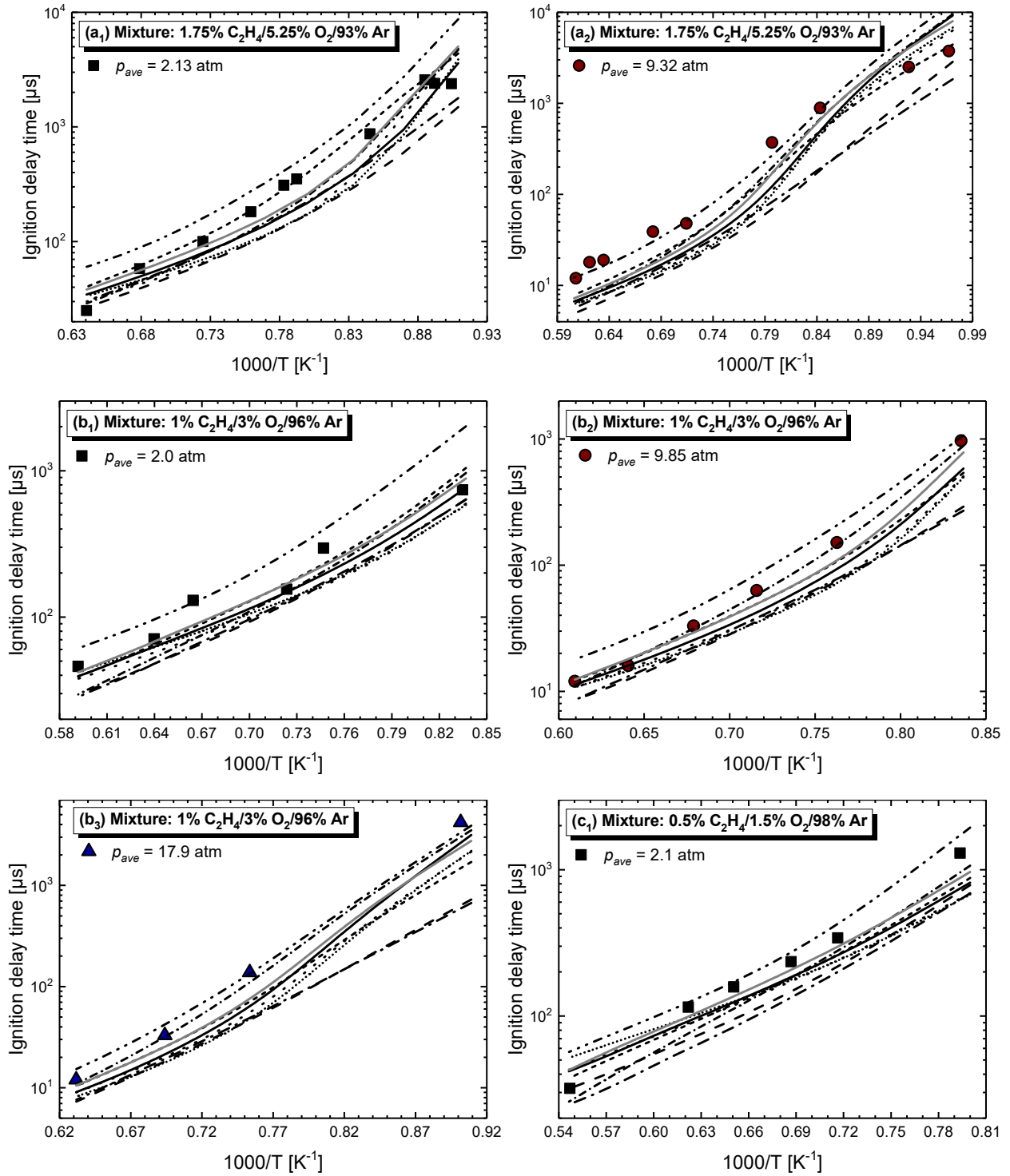


Figure S7: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.8 Saxena et al. experimental data[8]



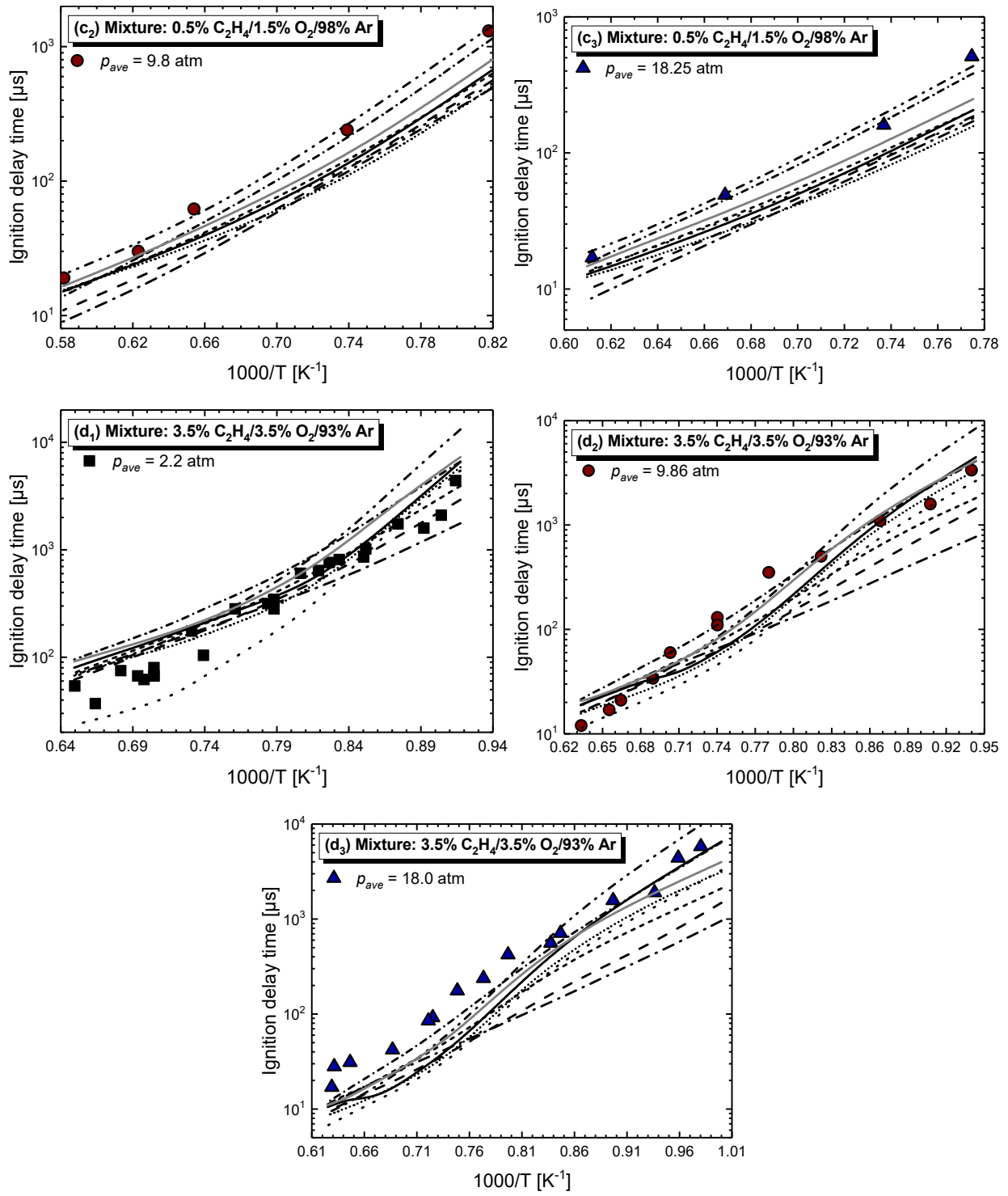


Figure S8: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.9 Davidson et al. experimental data[9]

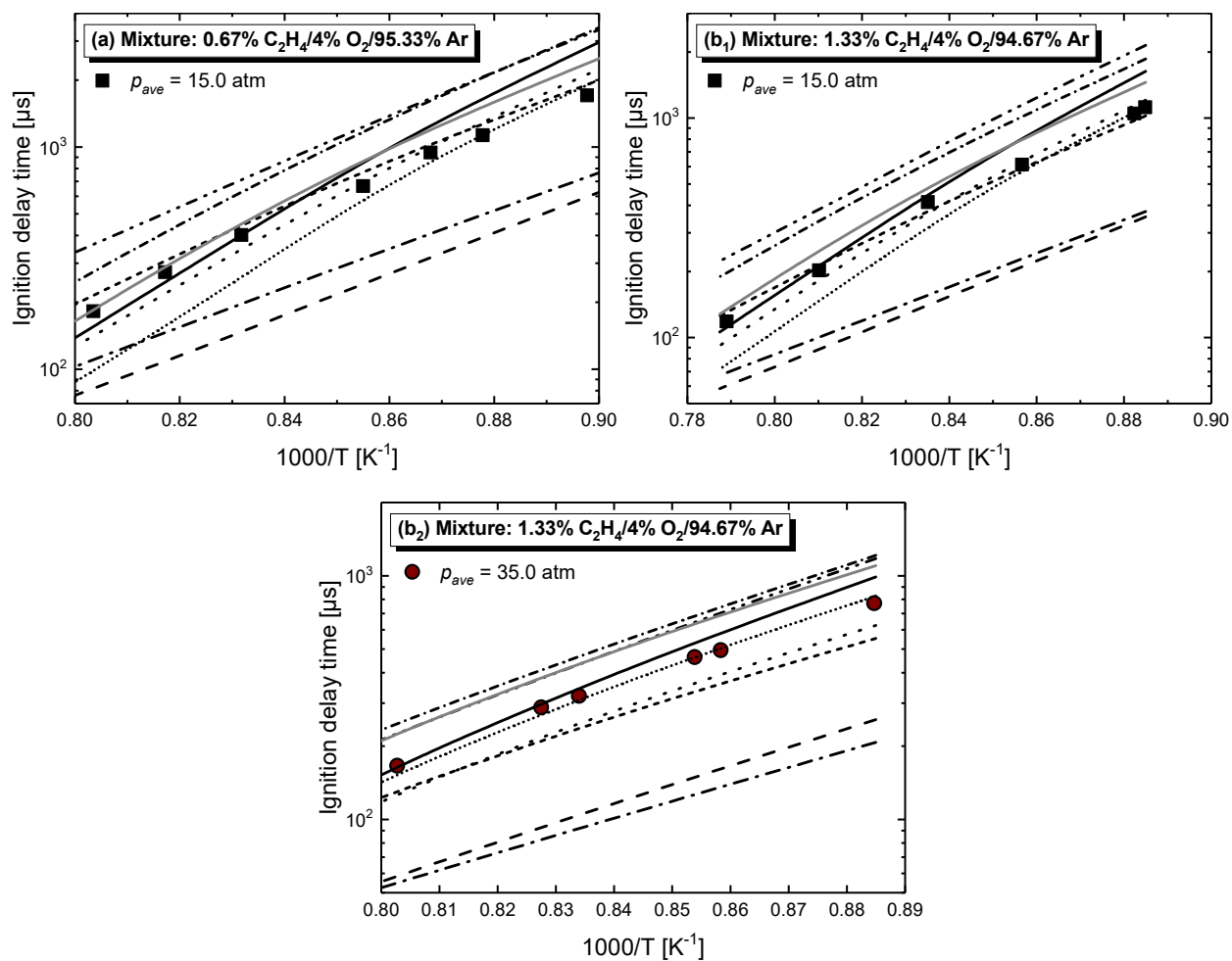
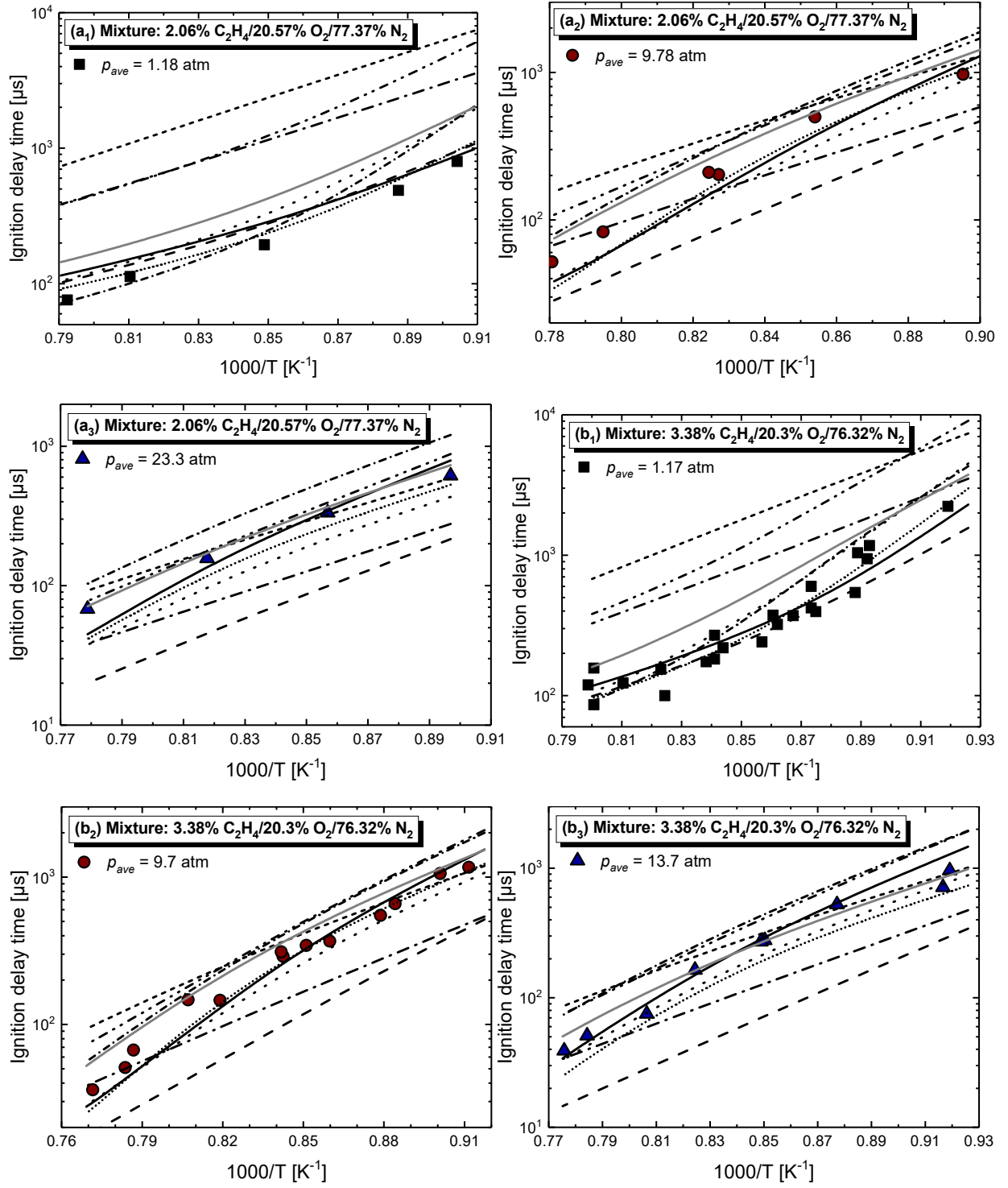


Figure S9: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.10 Kopp et al. experimental data[10]



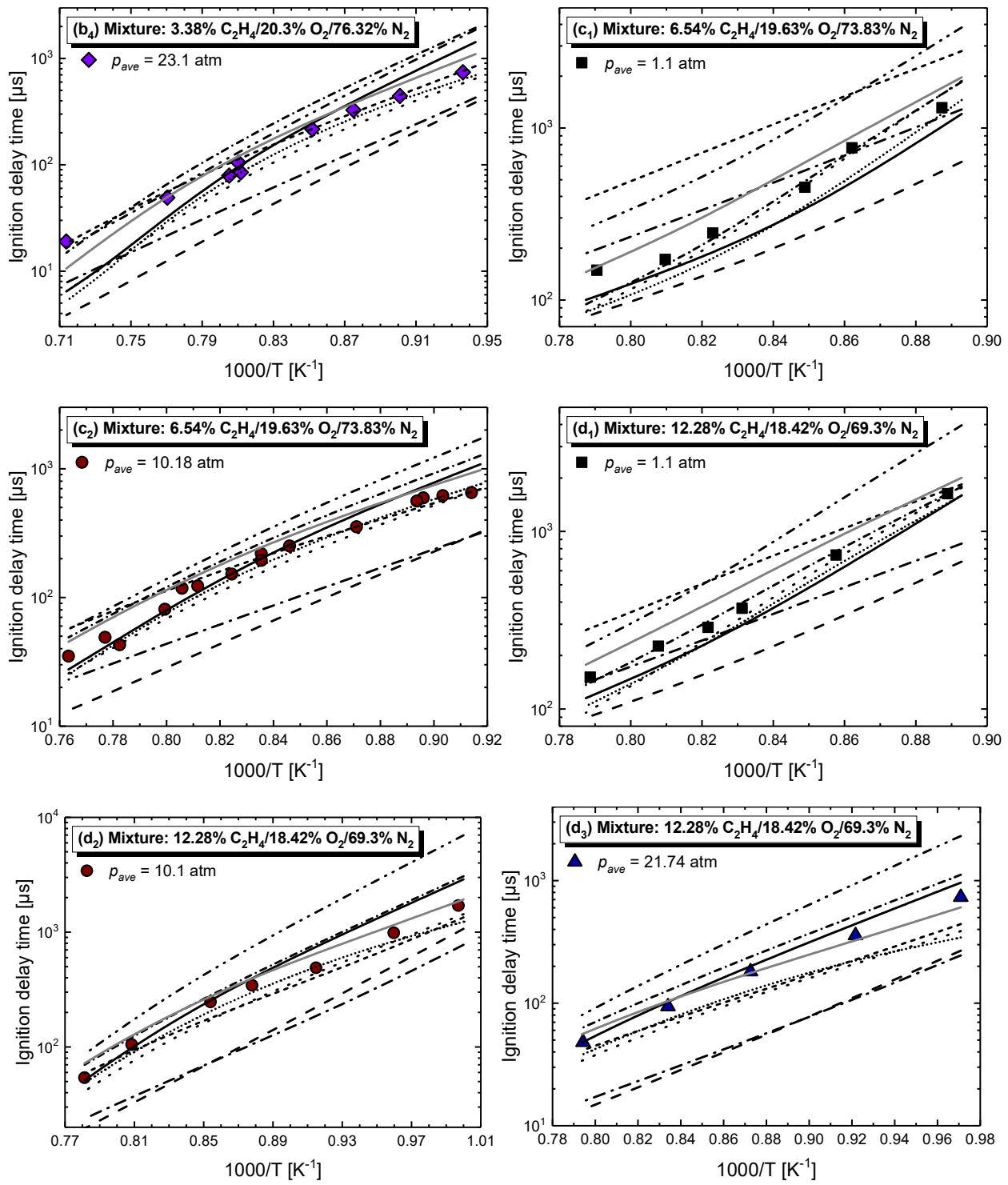


Figure S10: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.11 Mathieu et al. experimental data[11]

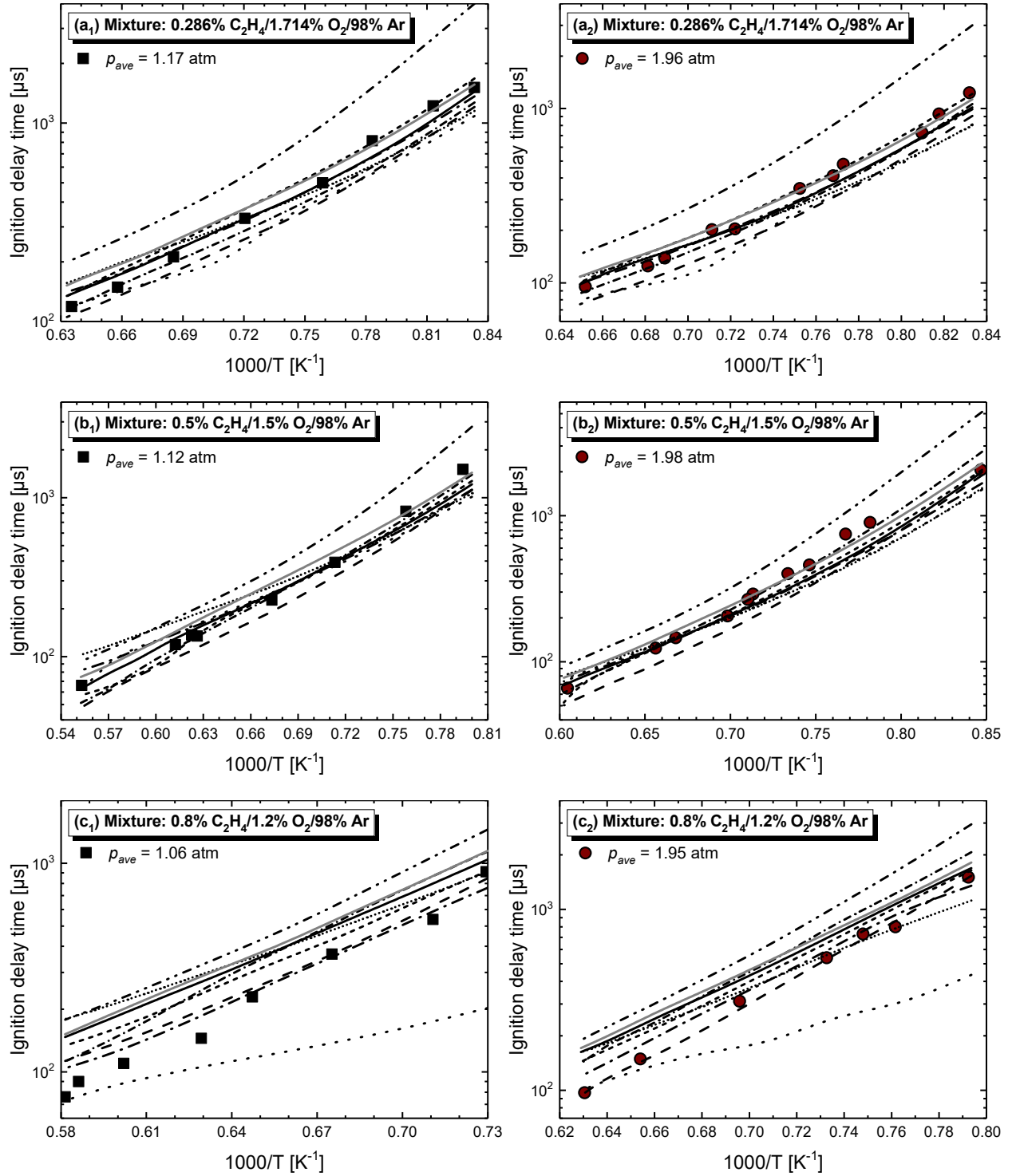


Figure S11: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.12 Xiong et al. experimental data[12]

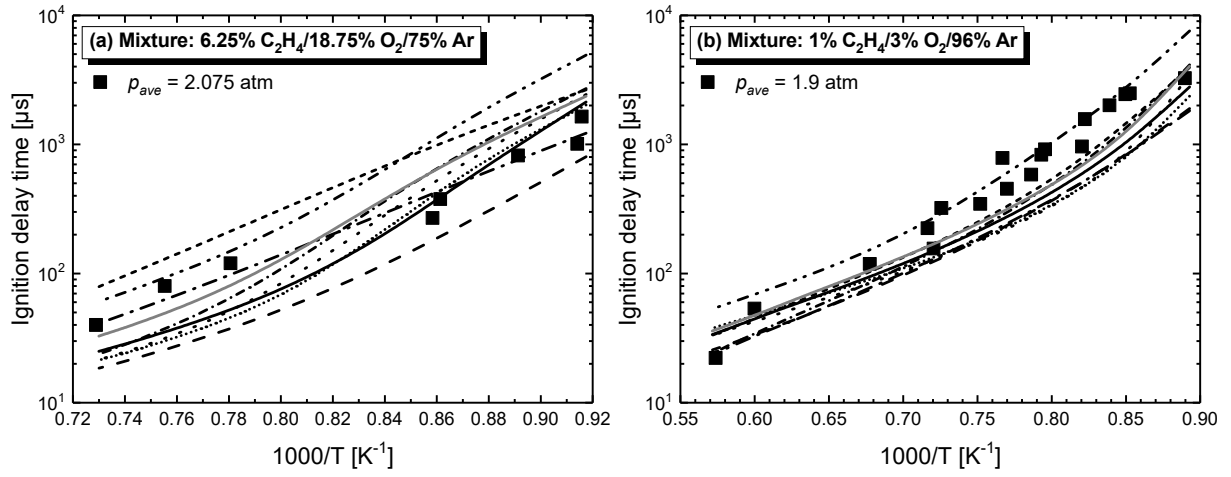


Figure S12: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.13 Shao et al. experimental data[13]

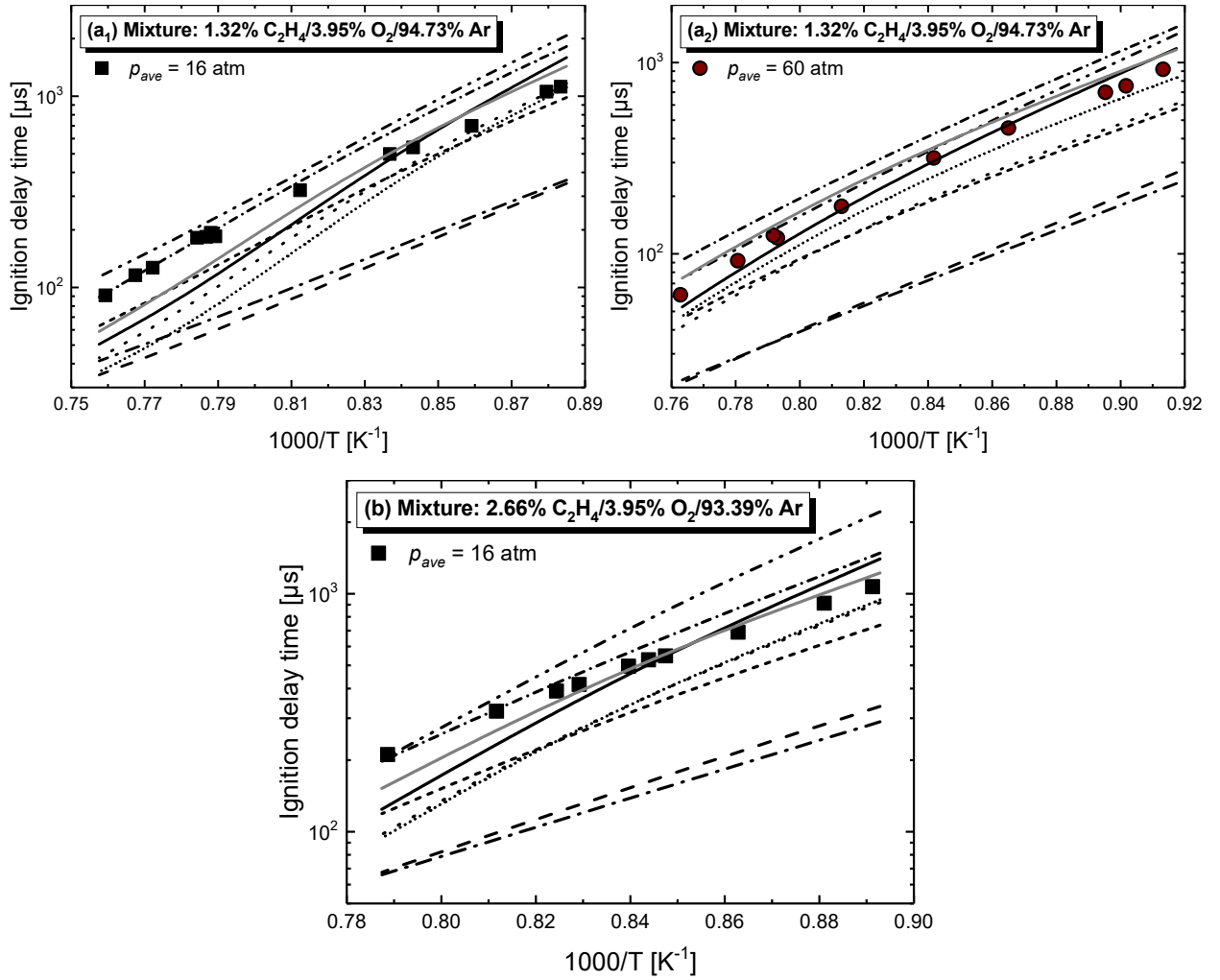


Figure S13: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.14 Baigmohammadi *et al.* experimental data[14]

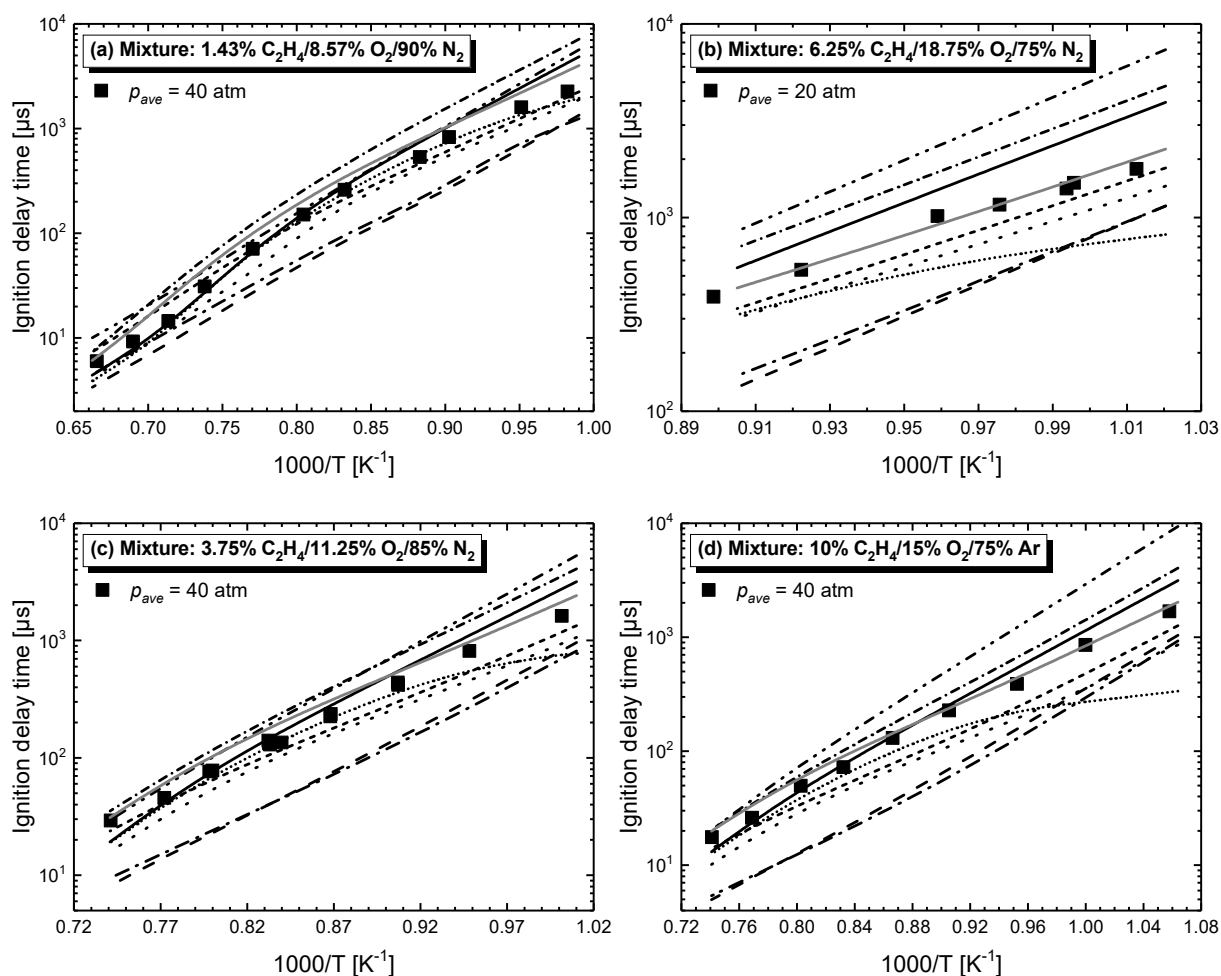
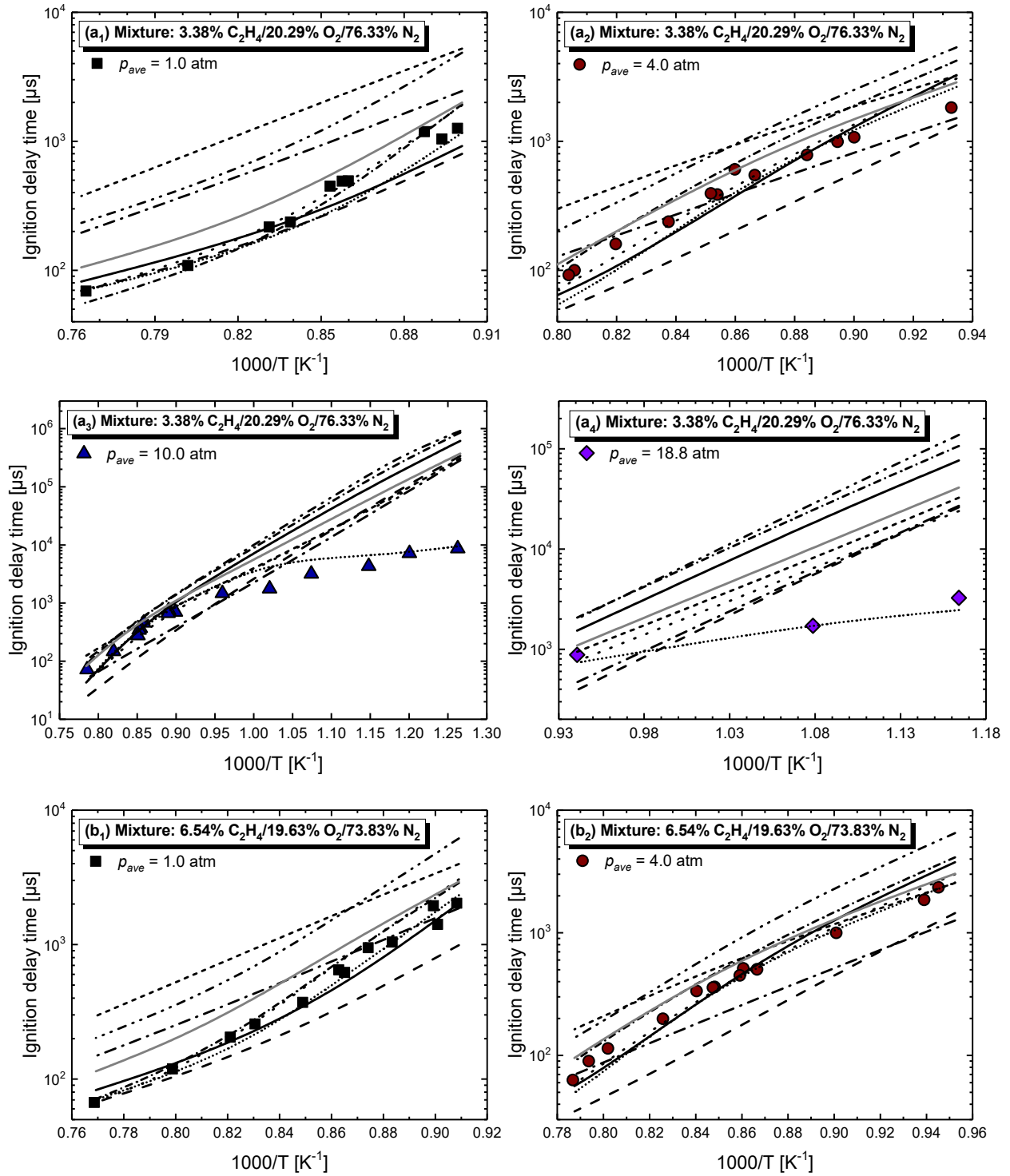


Figure S14: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.15 Yang et al. experimental data[15]



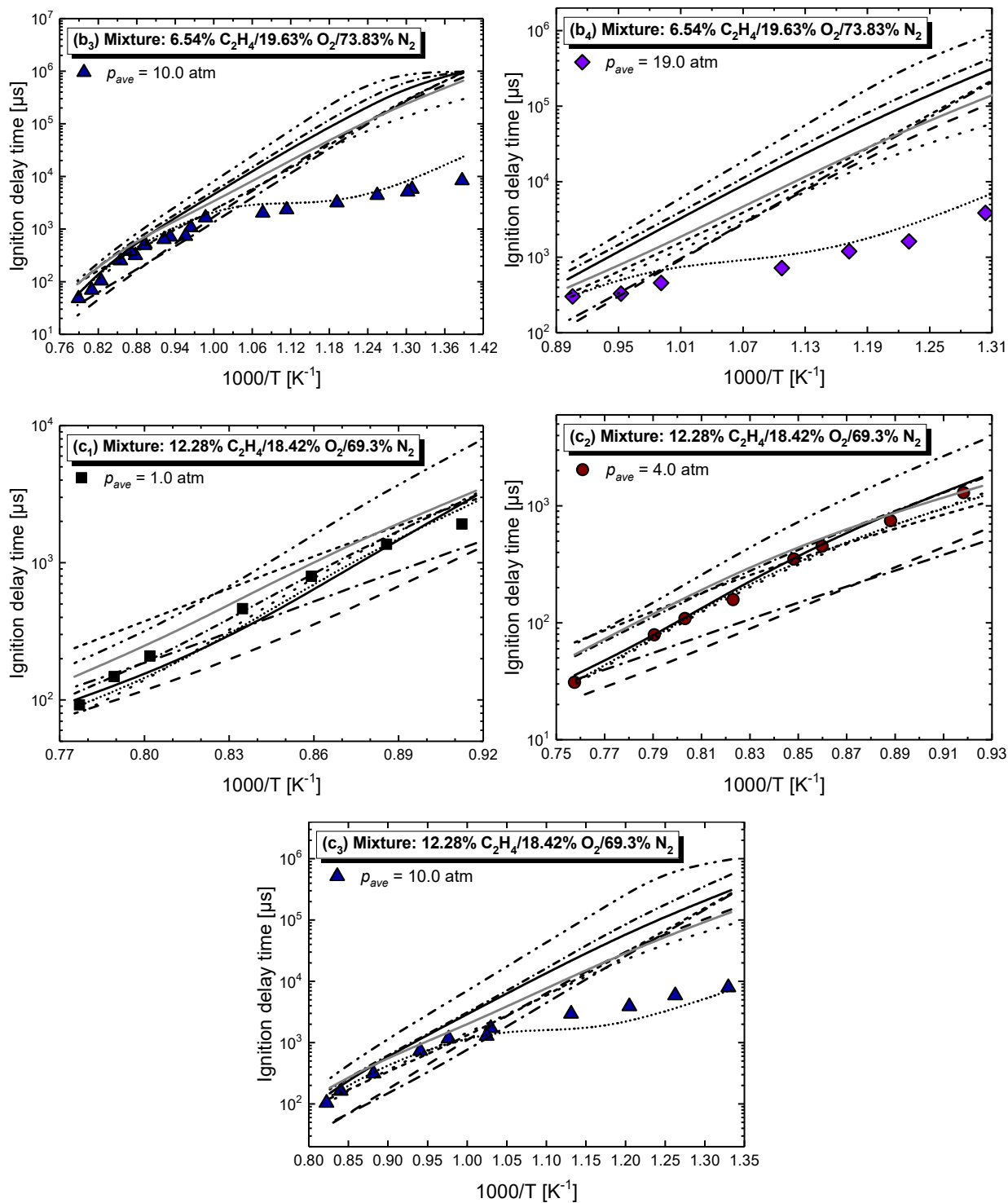


Figure S15: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.16 Xiong et al. experimental data[16]

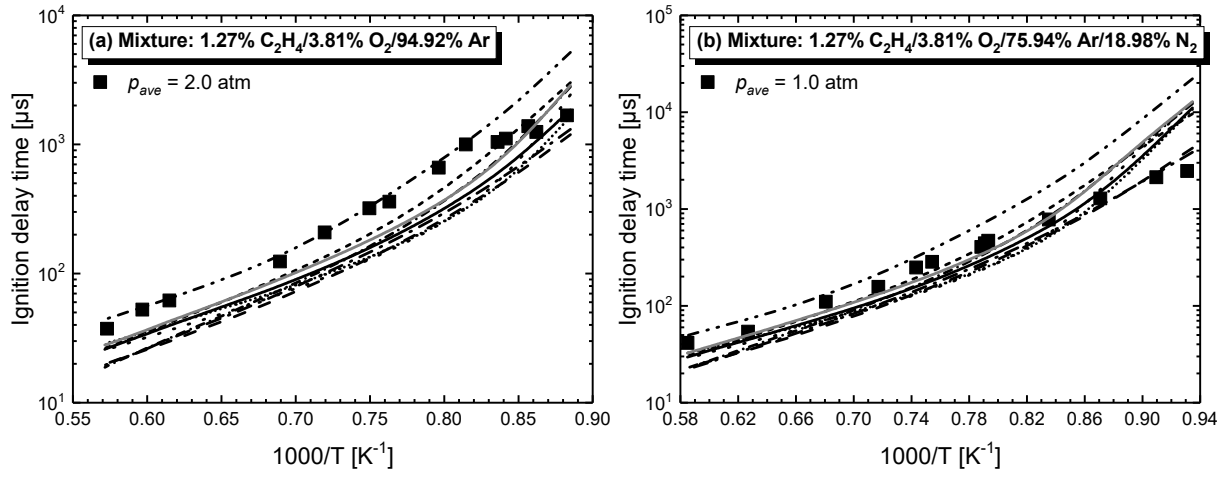


Figure S16: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.1.17 Dong et al. experimental data[17]

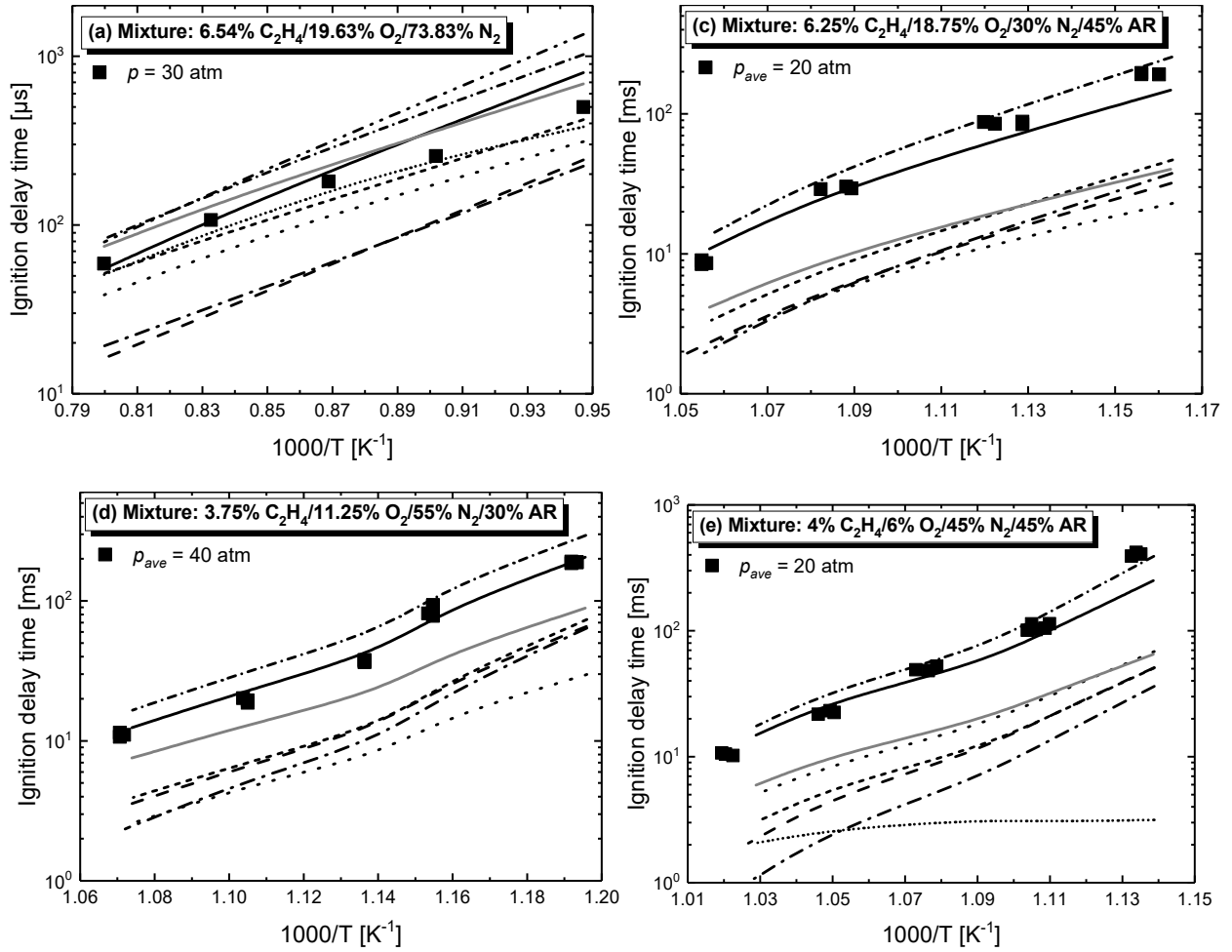


Figure S17: Shock tube ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.2 Rapid compress machine ignition delay times of ethylene

1.2.1 Baigmohammadi et al. experimental data[14]

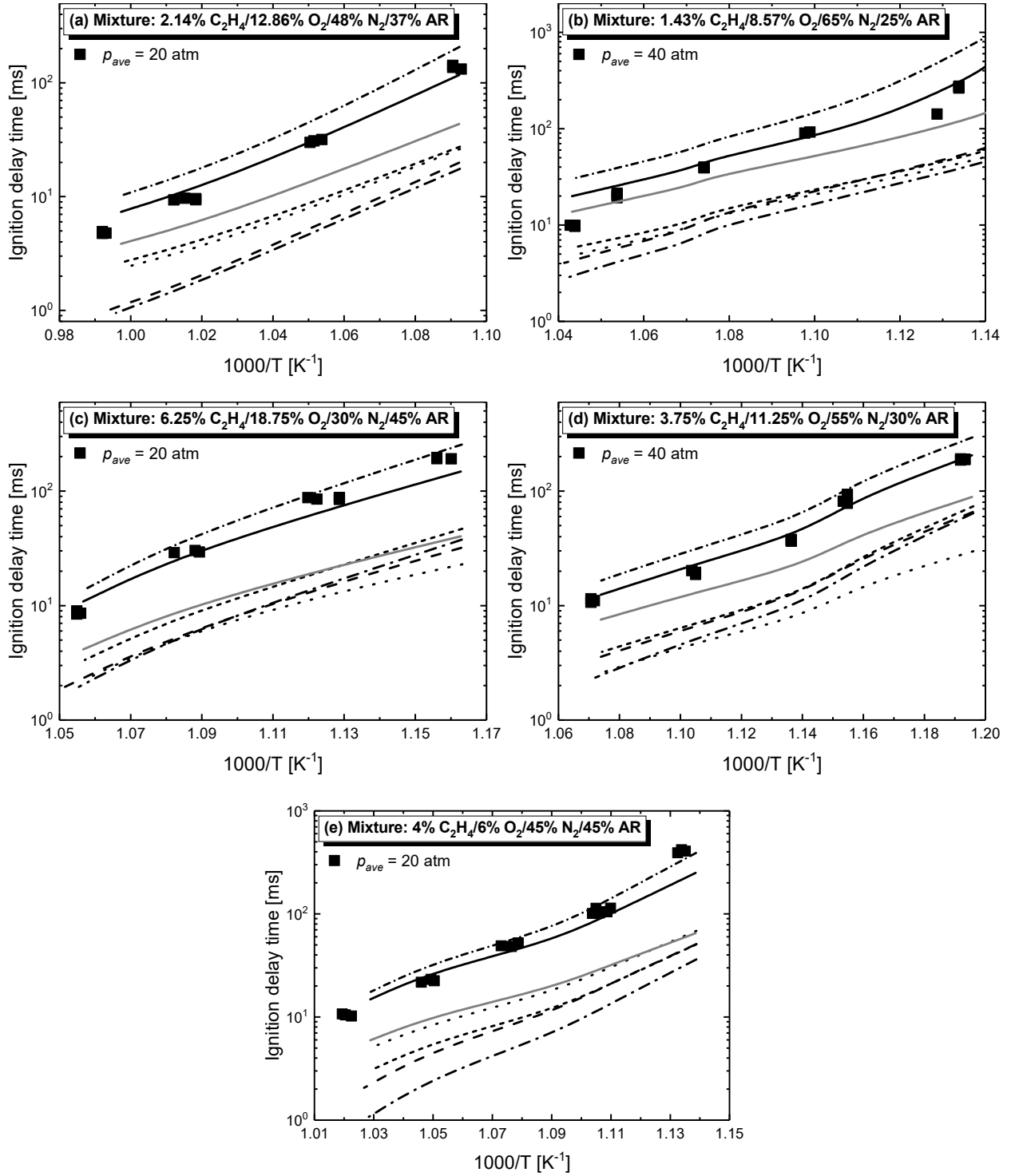


Figure S18: Rapid compress machine ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

1.2.2 Dong et al. experimental data[17]

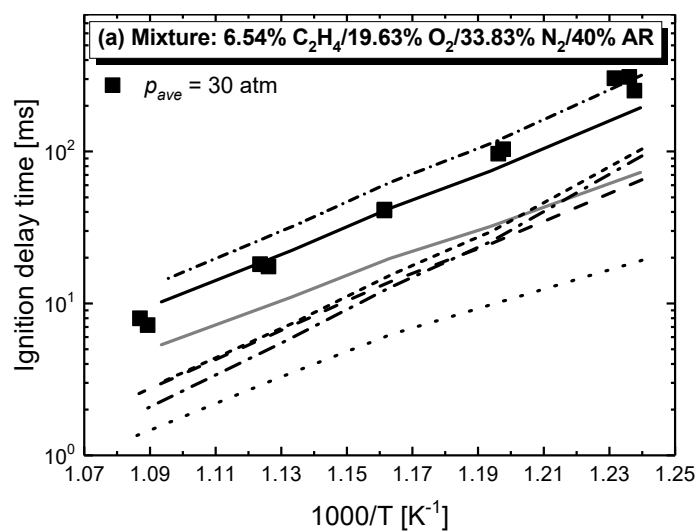


Figure S19: Rapid compress machine ignition delay times for ethylene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

2. Mechanism performance for propene

2.1 Shock tube ignition delay times of ethylene

2.1.1 Burcat and Radhakrishnan experimental data[18]

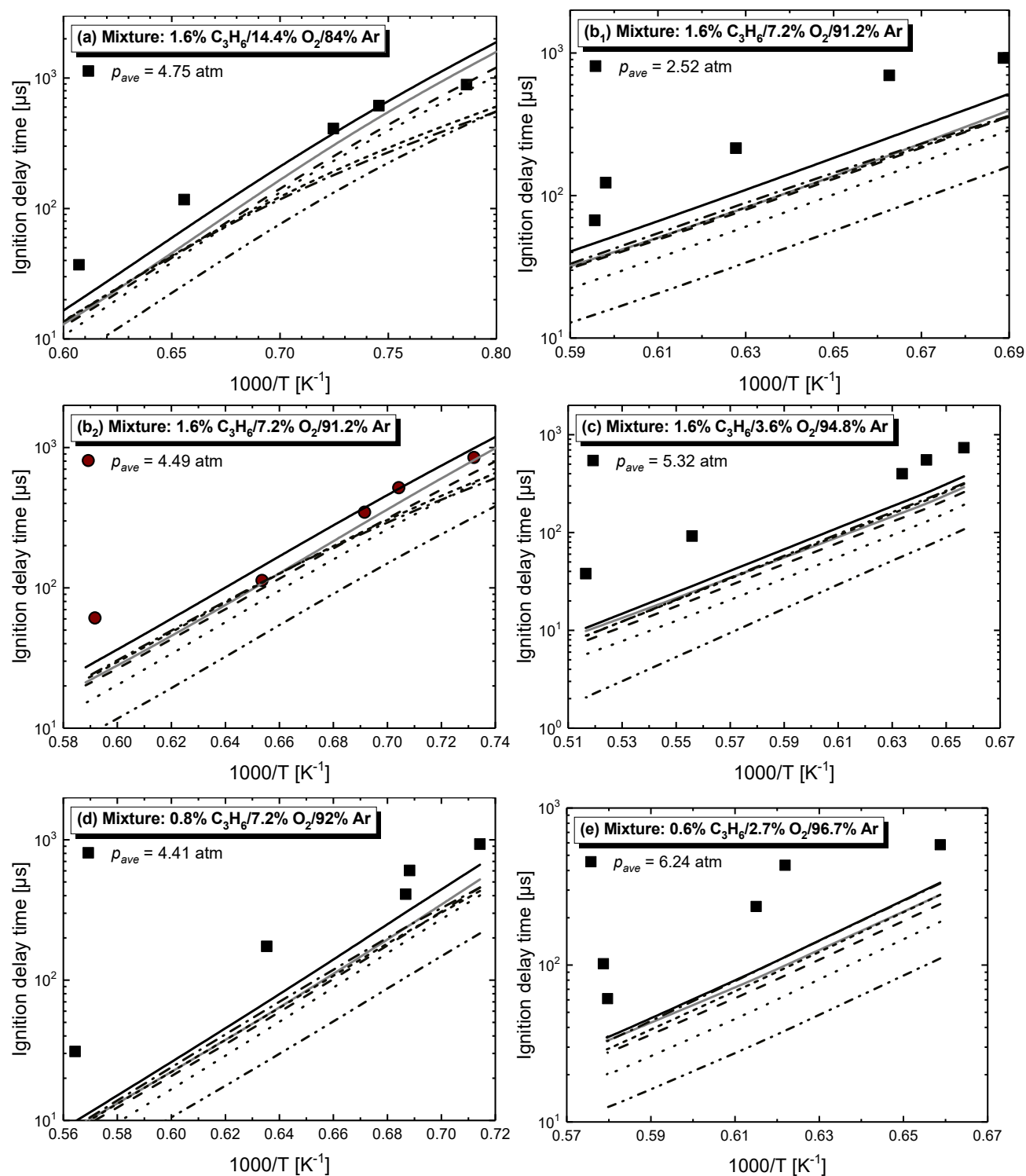


Figure S20: Shock tube ignition delay times for propene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

2.1.2 Qin et al. experimental data[19]

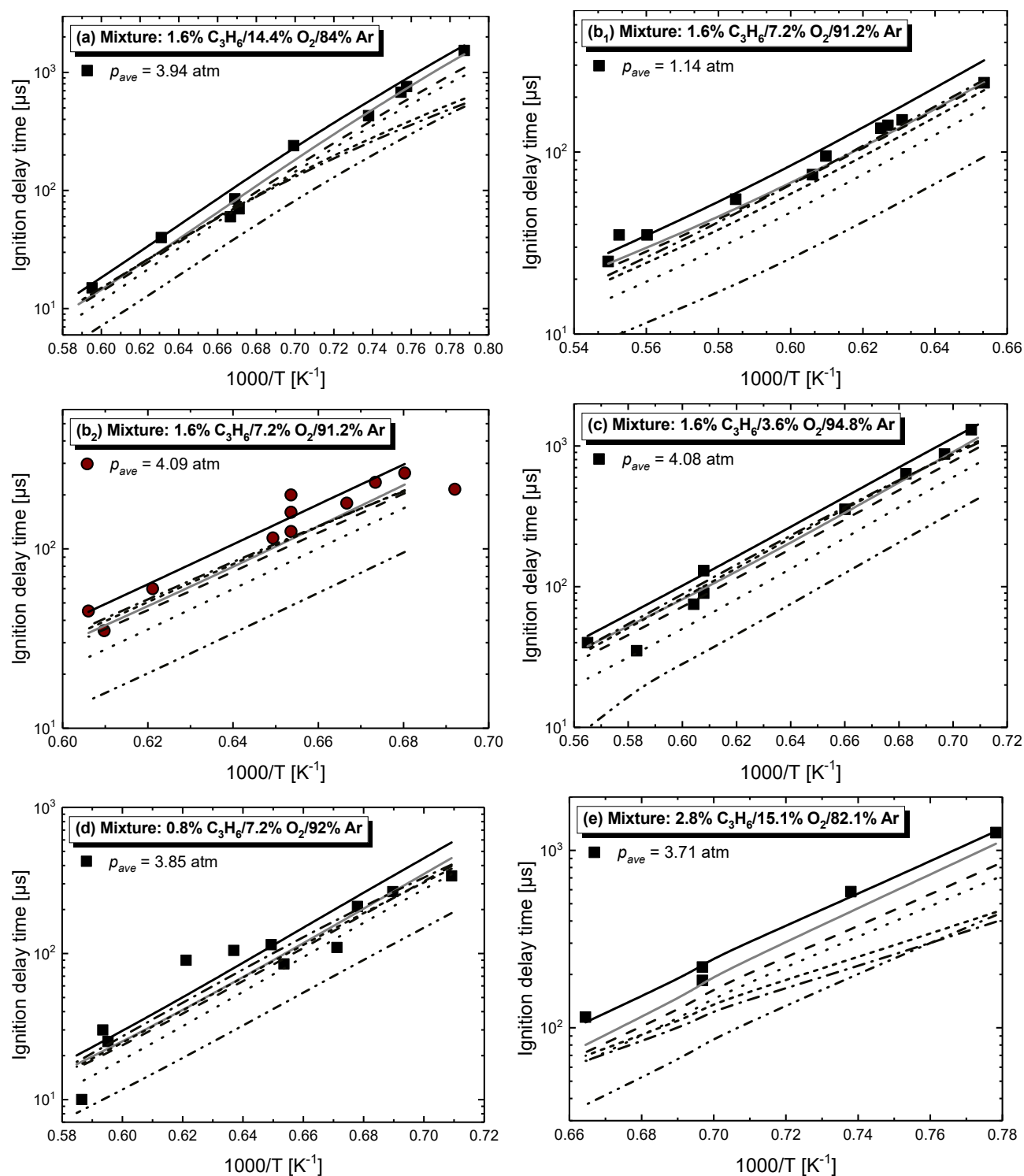
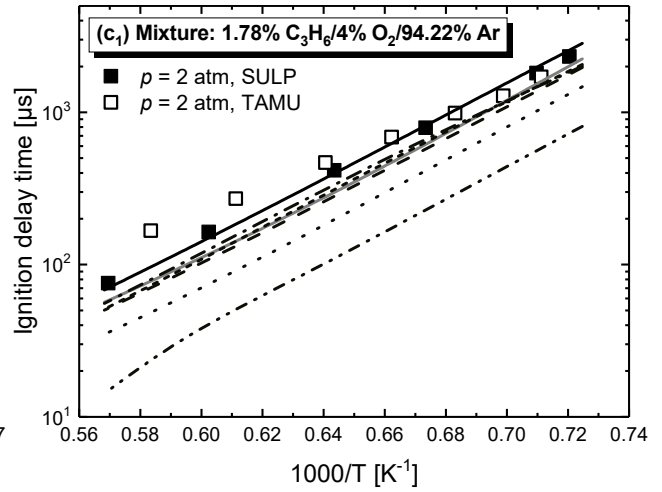
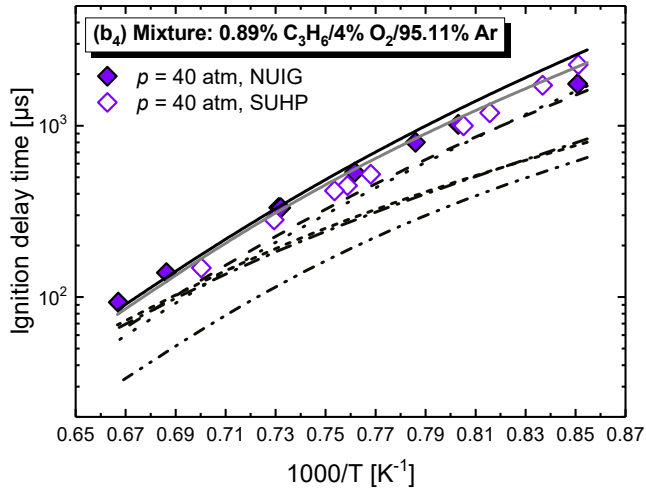
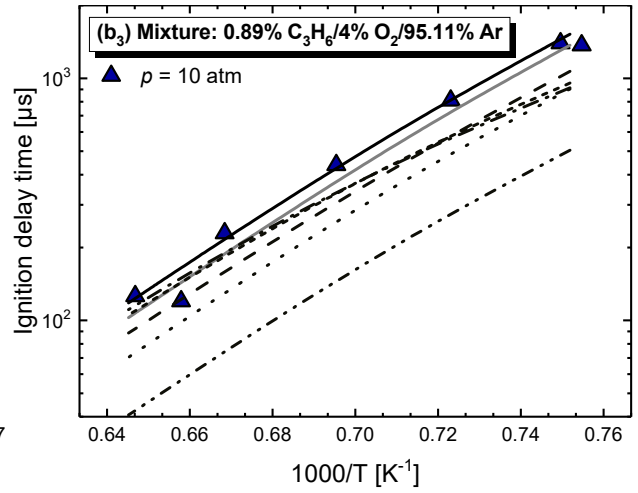
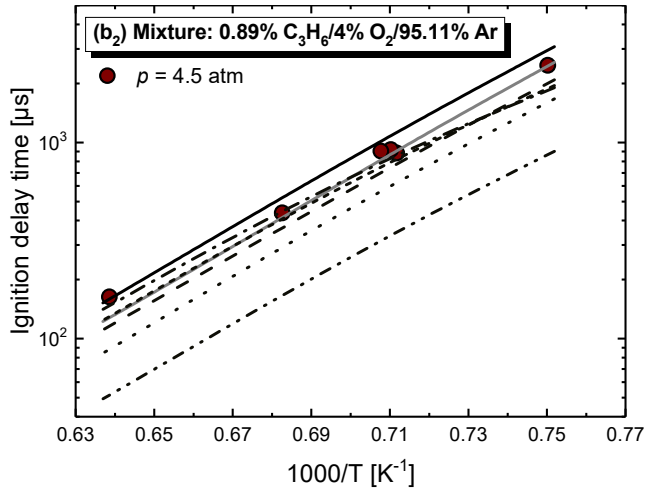
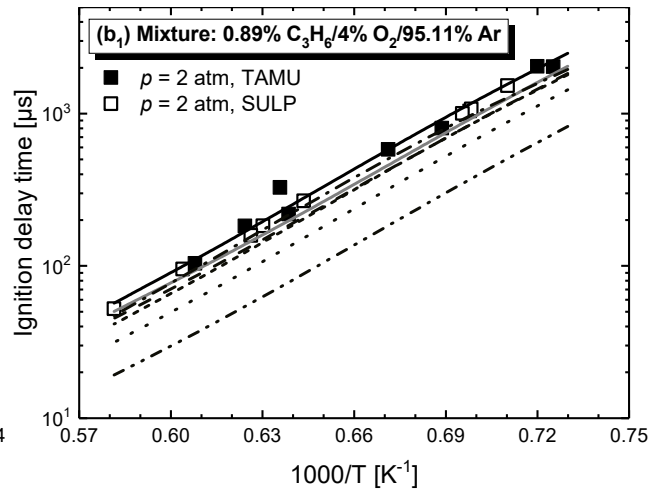
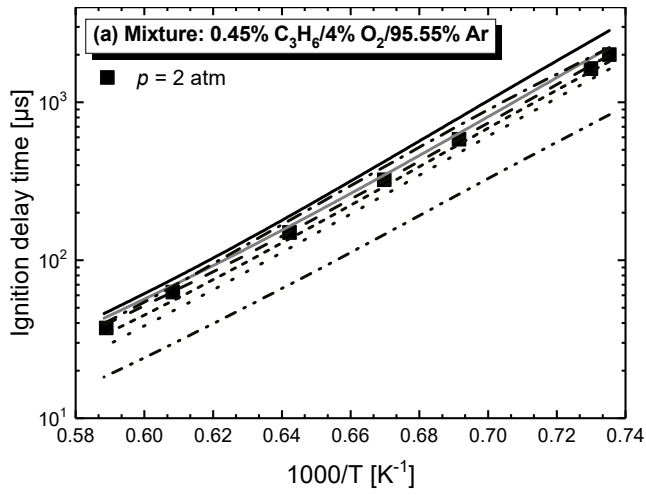


Figure S21: Shock tube ignition delay times for propene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

2.1.3 Burke et al. experimental data[20]

(1) Fuel in diluent



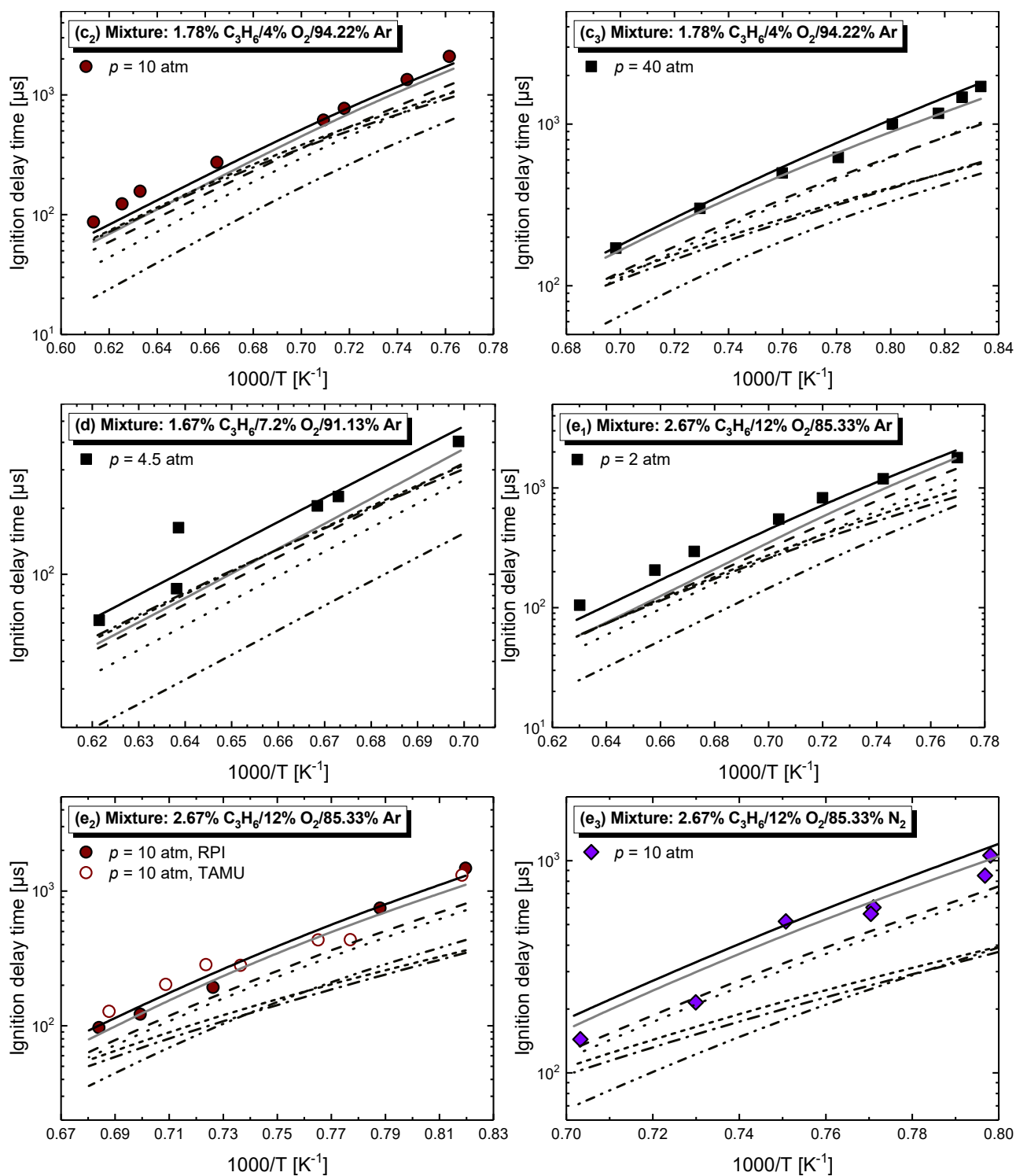
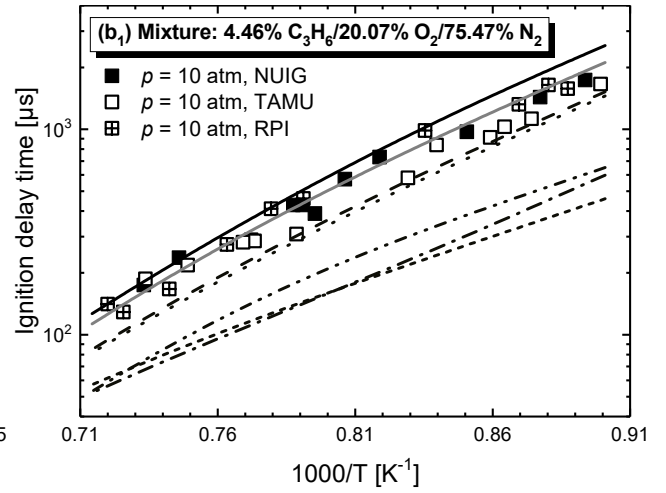
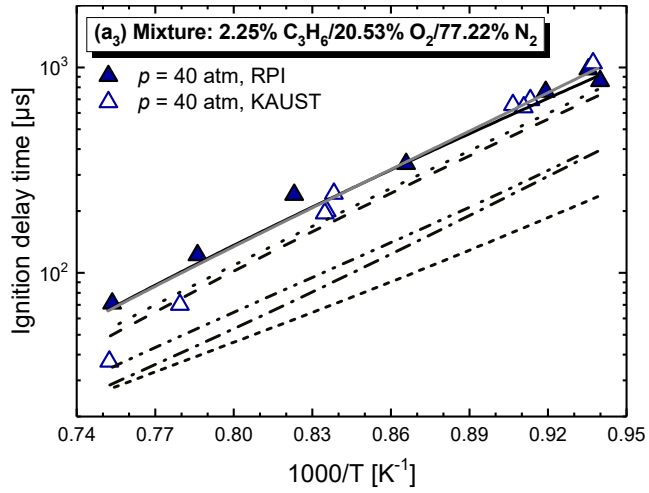
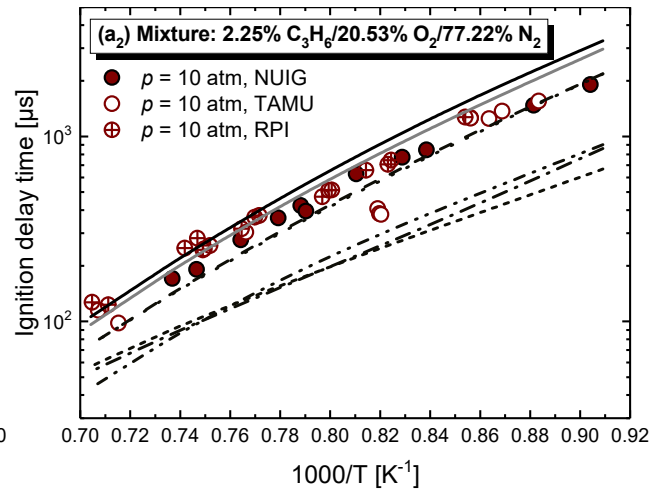
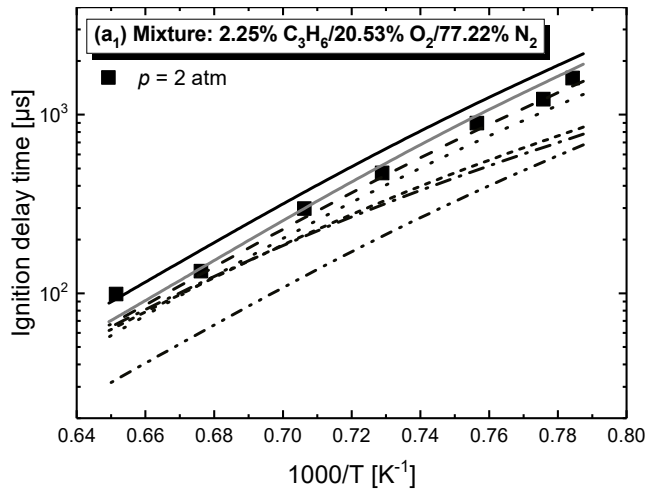


Figure S22: Shock tube ignition delay times for propene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

(2) Fuel in air



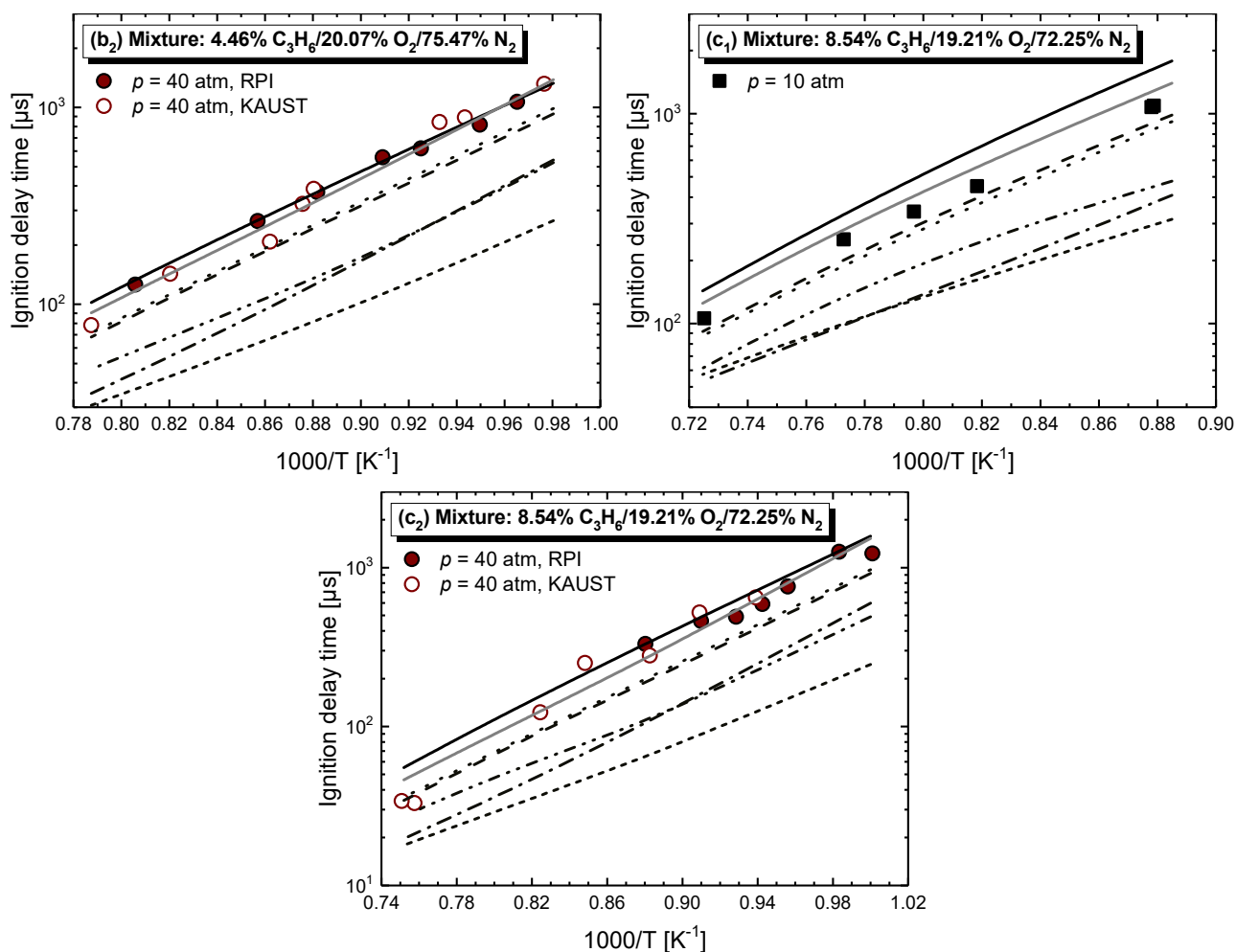


Figure S23: Shock tube ignition delay times for propene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

2.1.4 Shao et al. experimental data[13]

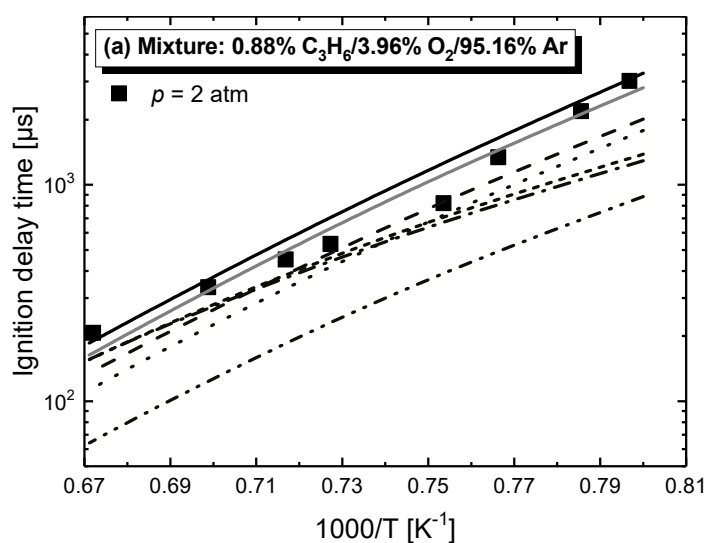


Figure S24: Shock tube ignition delay times for propene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

3. Mechanism performance for 1-butene

3.1 Shock tube ignition delay times of 1-butene

3.1.1 Heyberger et al. experimental data[21]

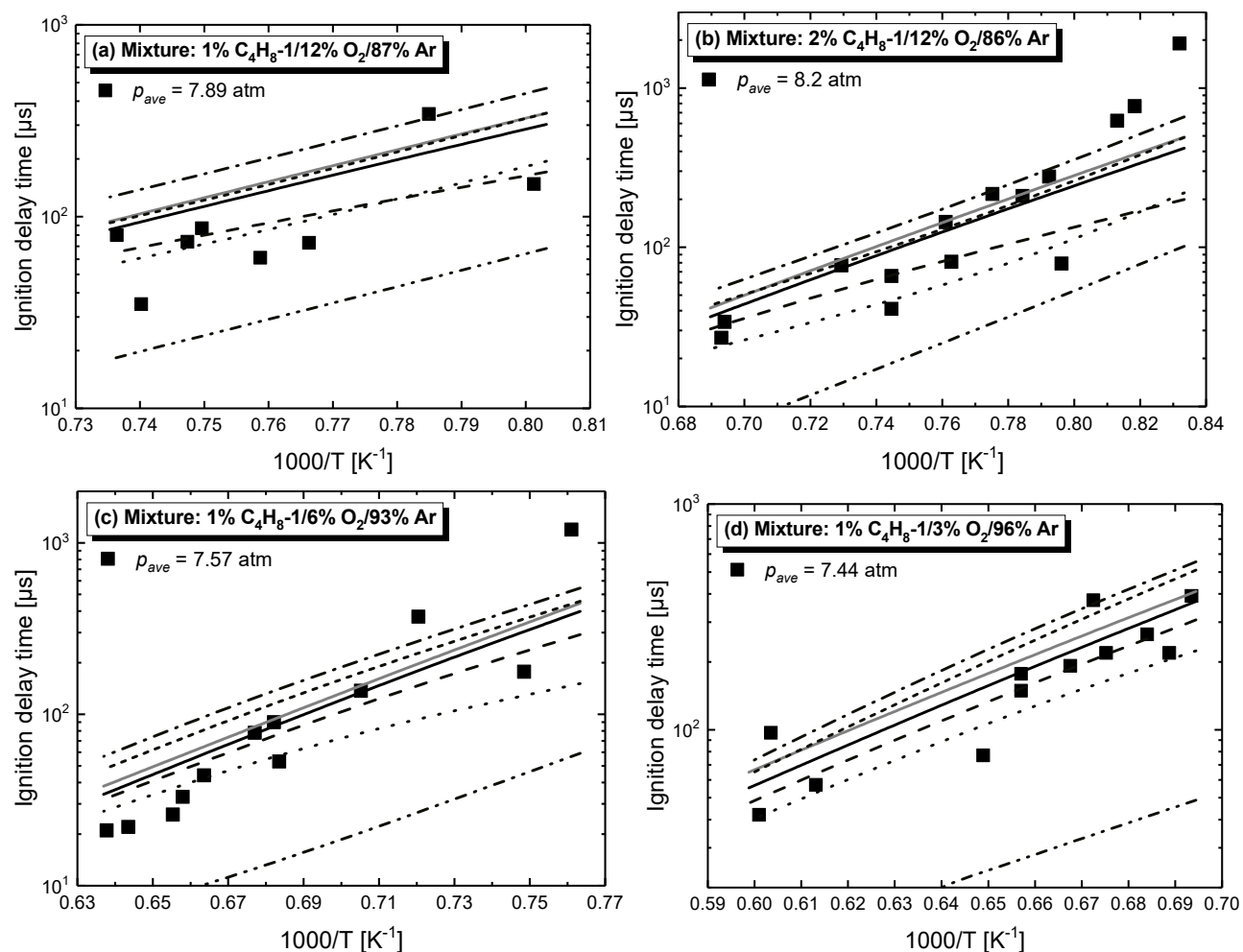
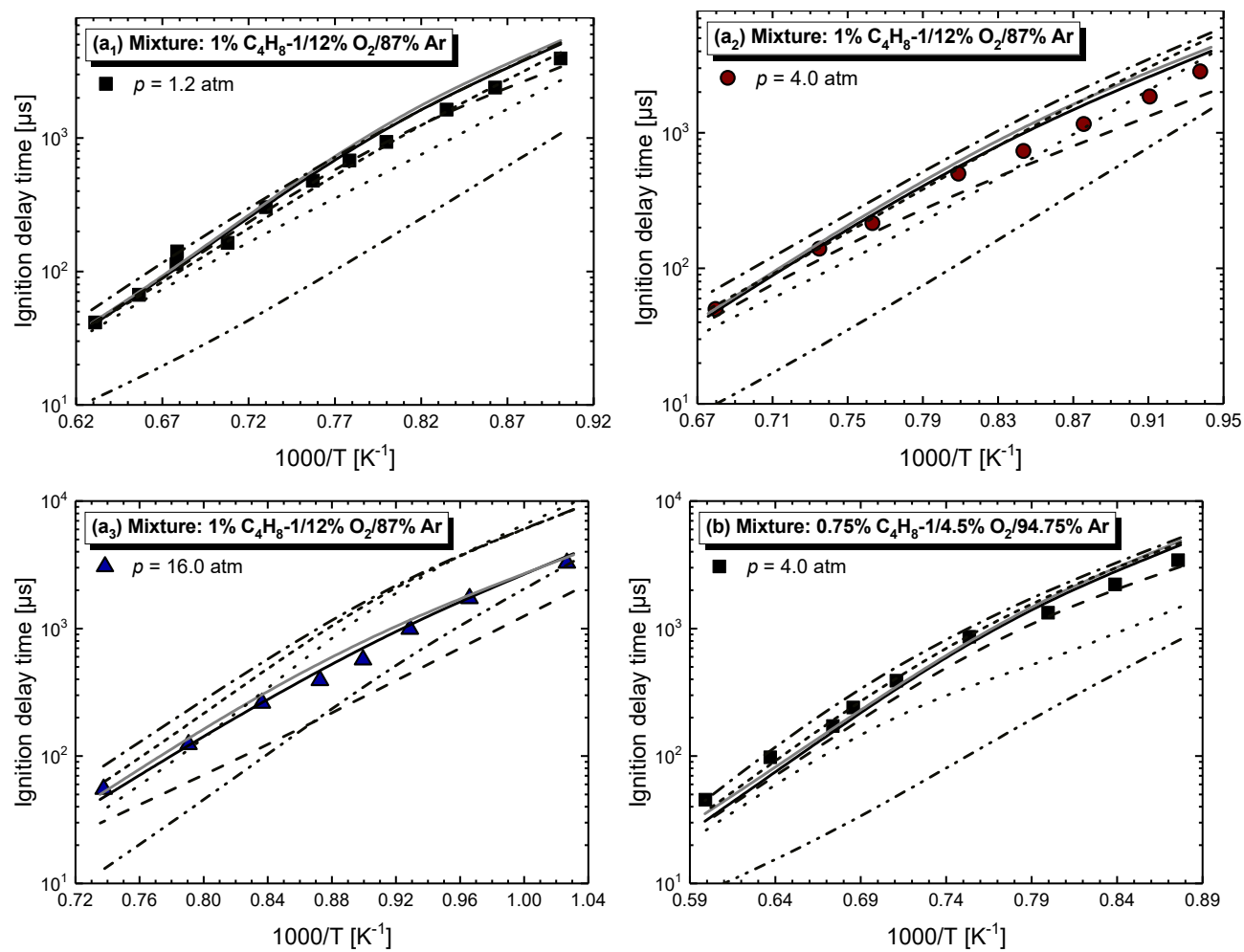


Figure S25: Shock tube ignition delay times for 1-butene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

3.1.2 Pan et al. experimental data[22]



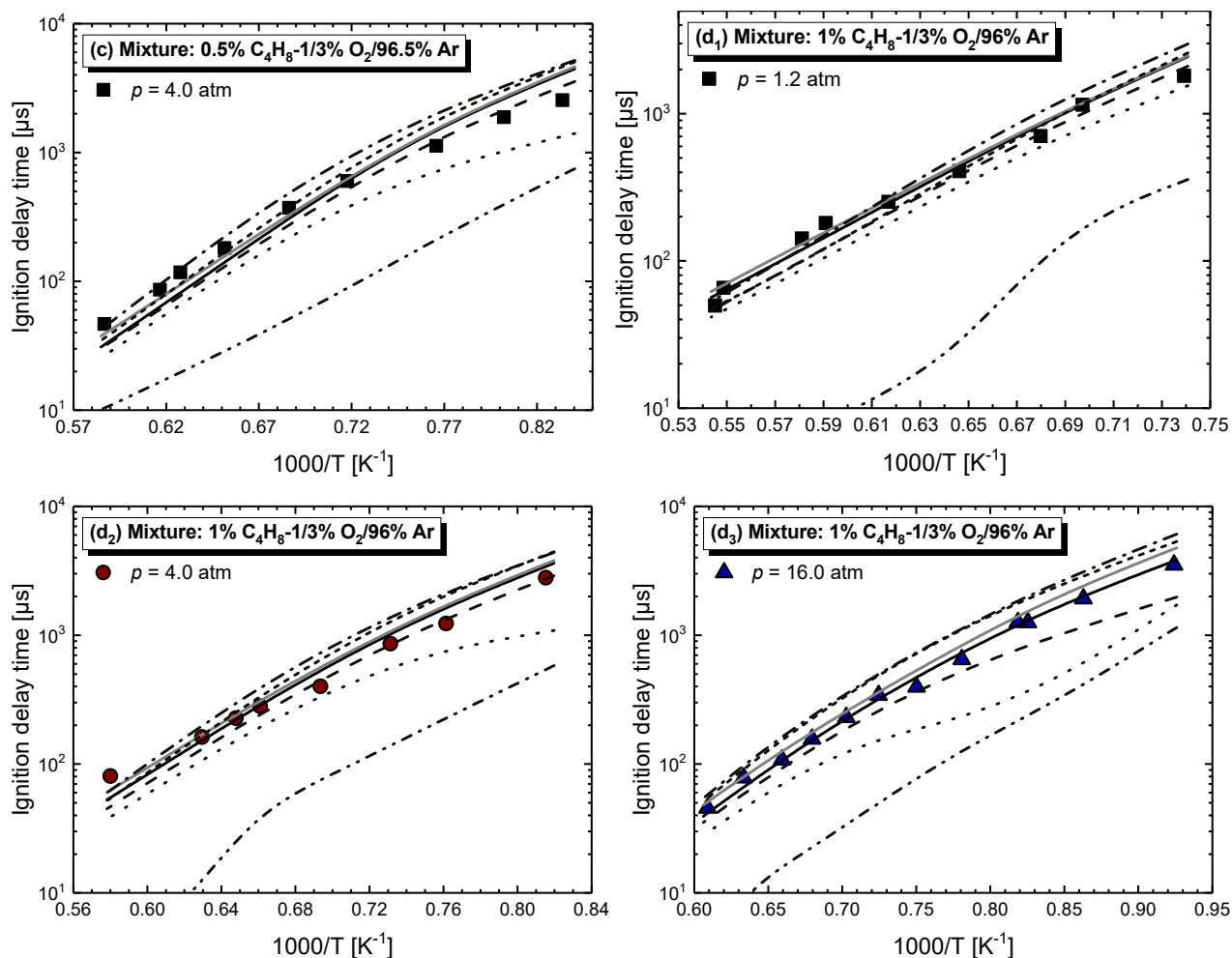
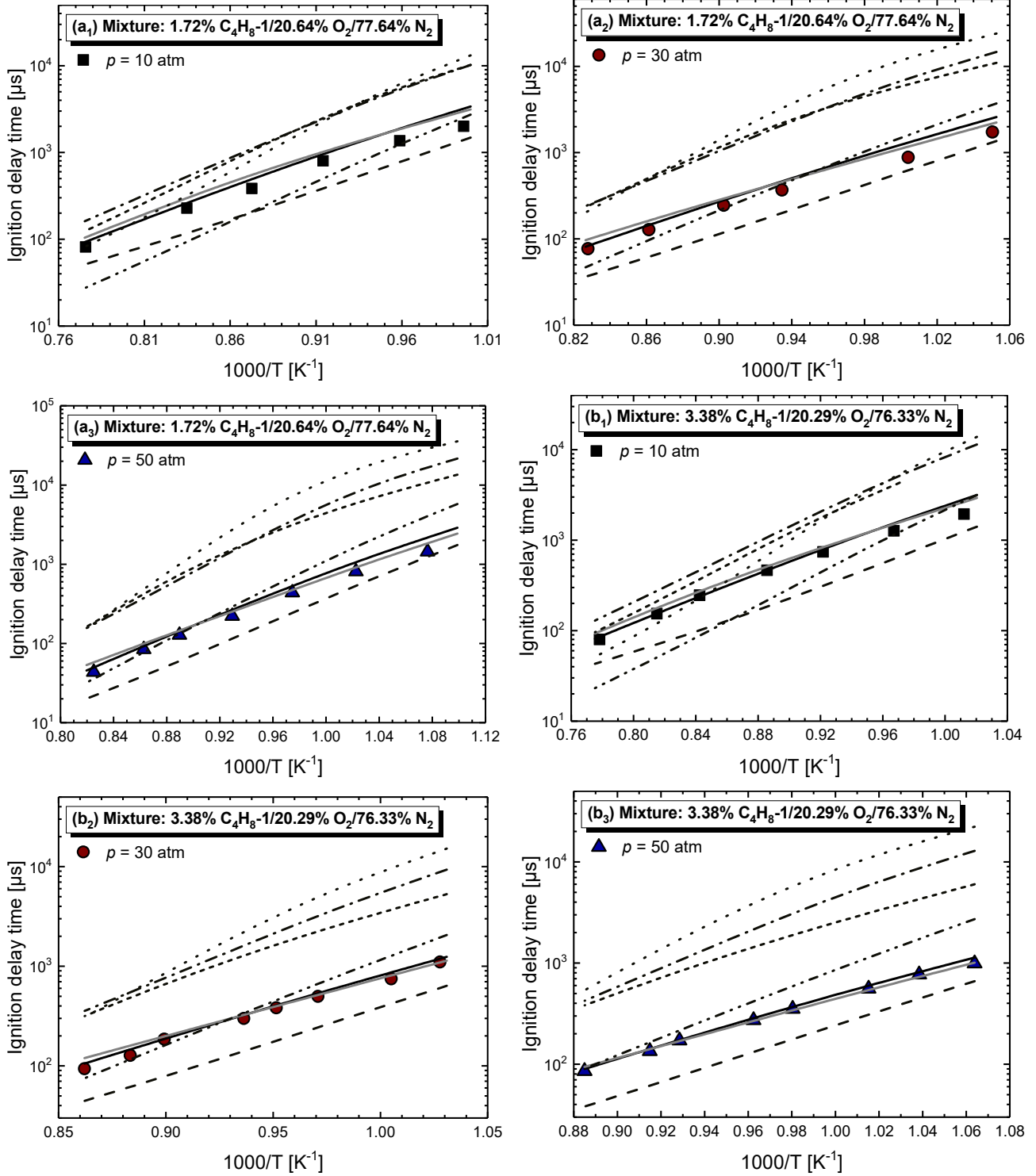


Figure S26: Shock tube ignition delay times for 1-butene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

3.1.3 Li et al. experimental data[23]



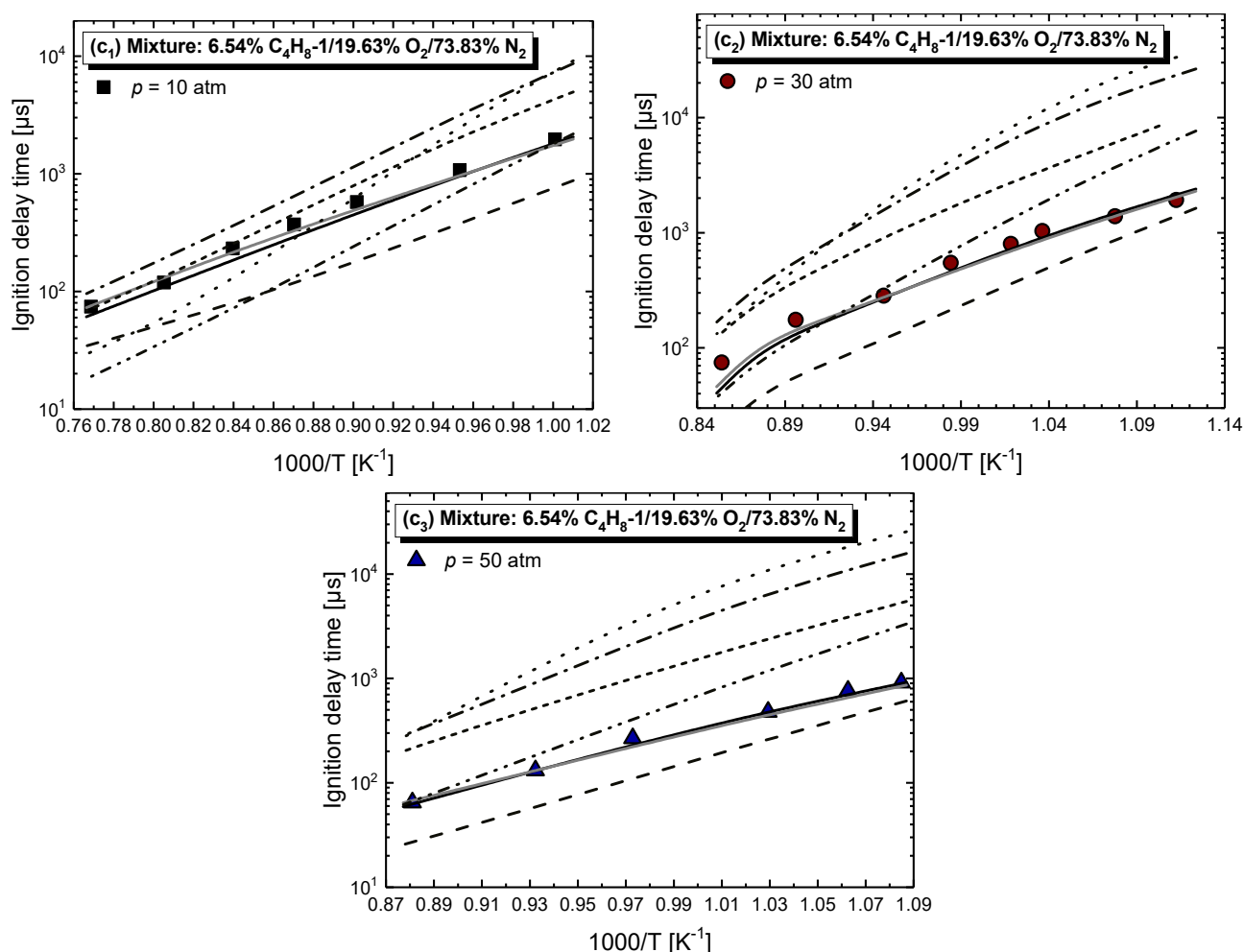


Figure S27: Shock tube ignition delay times for 1-butene mixtures. Symbols represent experimental data; lines denote model predictions with the selected mechanisms.

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