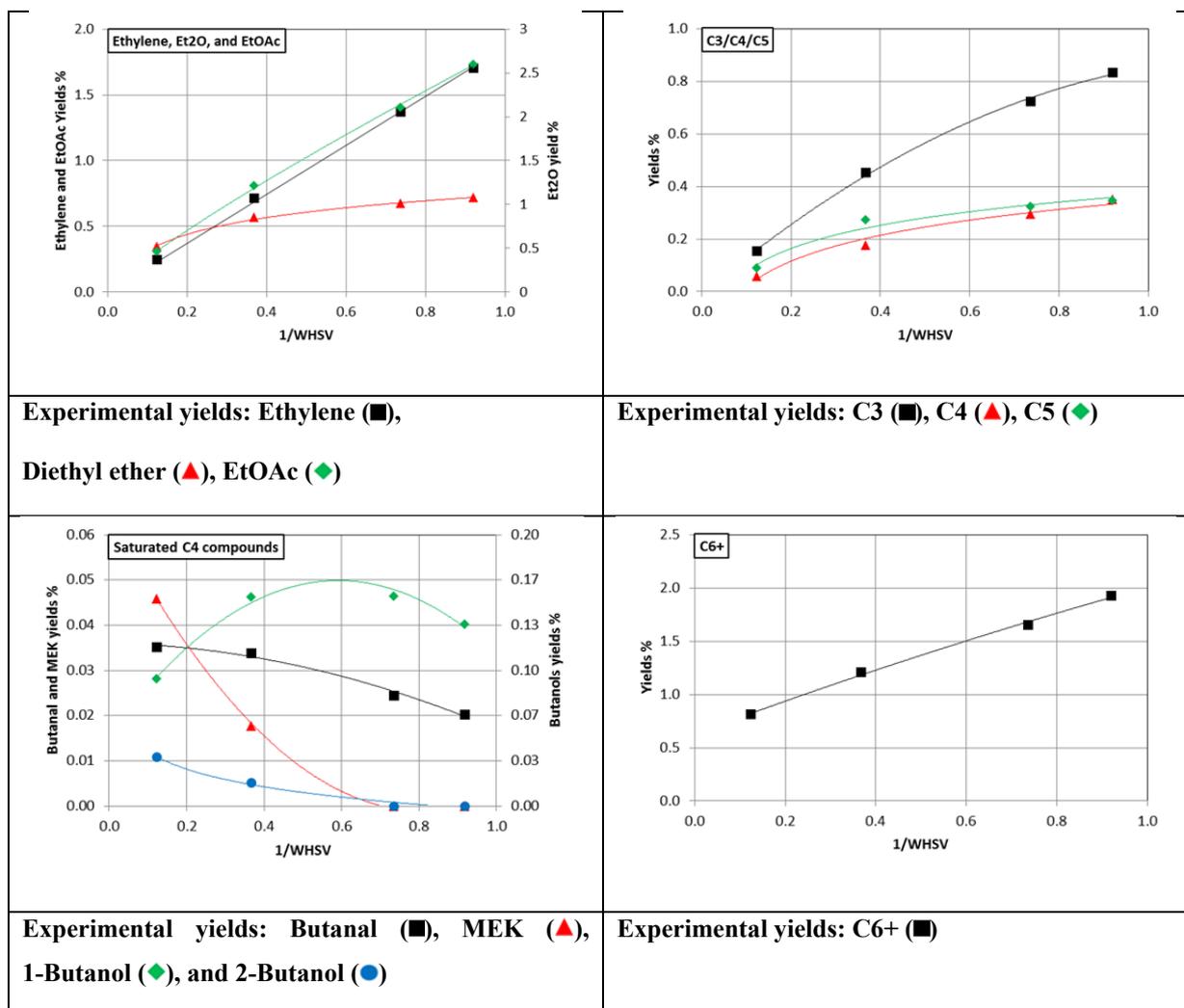


1 Products yields

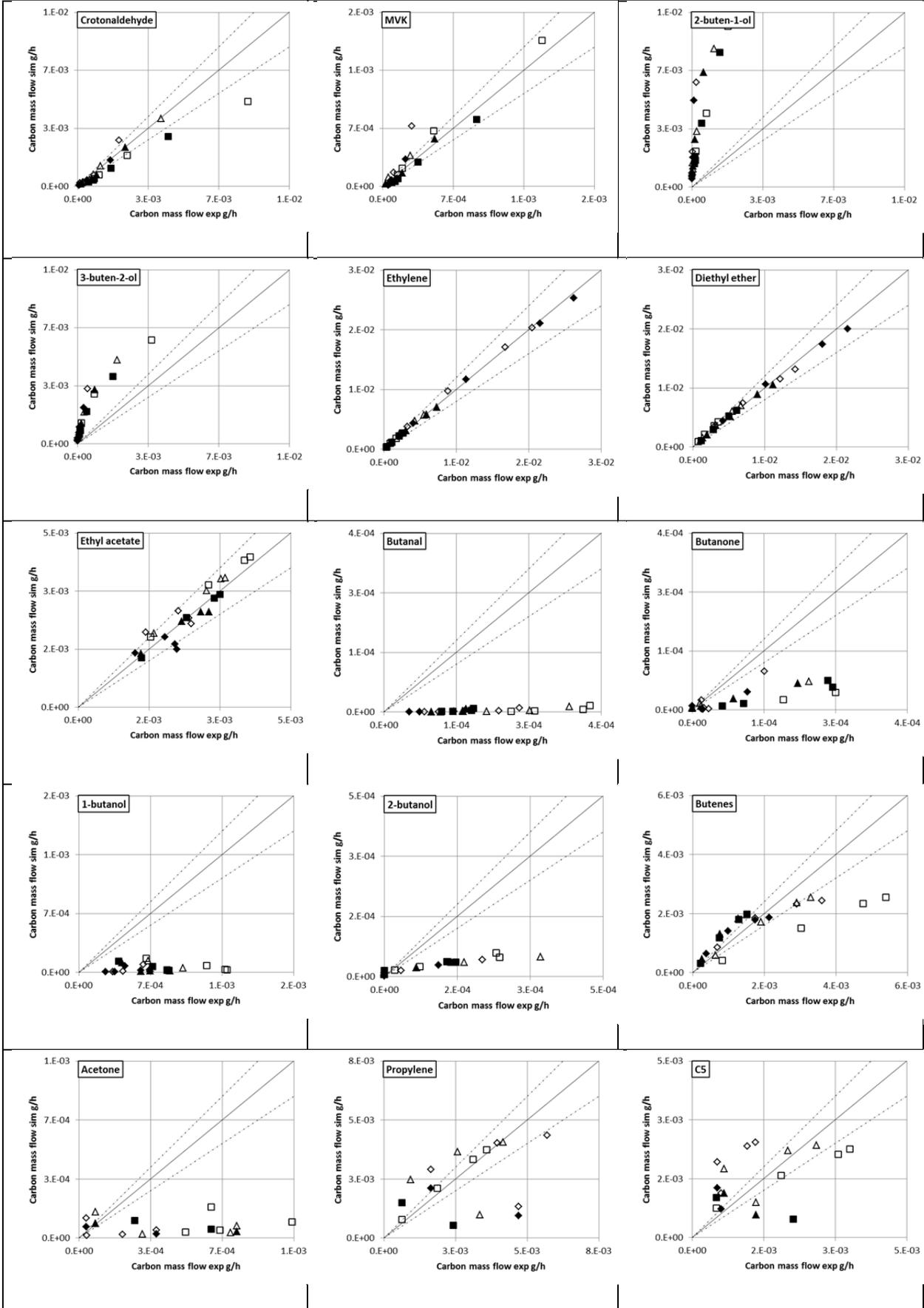
Operating conditions for all graphs herein below: T: 340 °C; EtOH/AcH ratio: 3.6

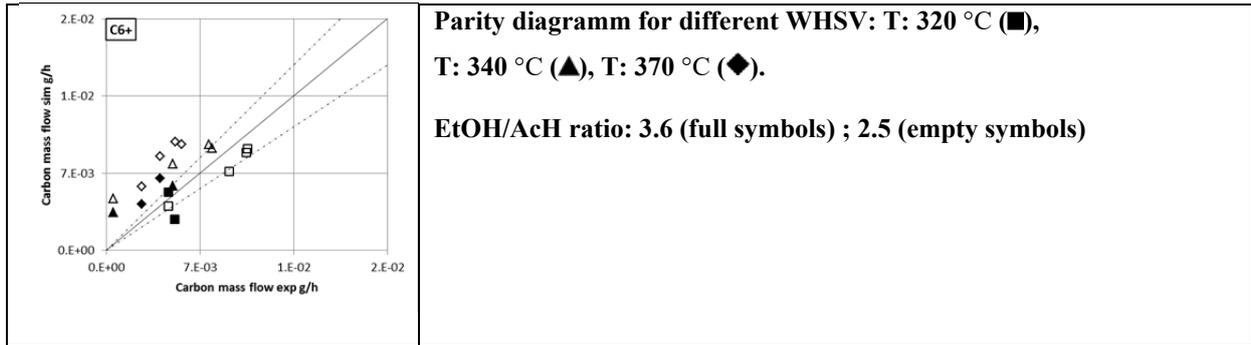
Lines are drawn to guide the eyes.



2 Parity diagrams

Parity diagrams of all components but Ethanol Acetaldehyde and Butadiene. Major side products are in good agreement (ethylene, Et₂O and EtOAc) as well as carbonyl intermediates at a ratio of 3.6.





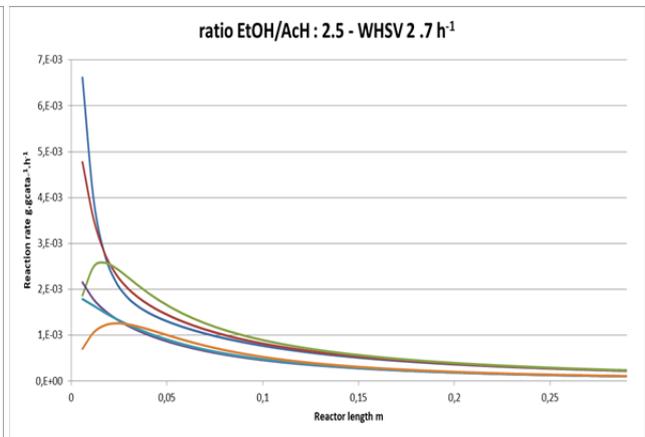
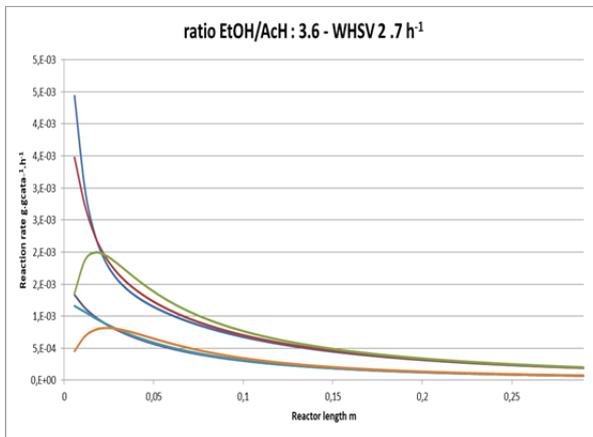
3 Reaction rates

$$\text{Kinetics laws: } r = k \left(\prod C_{reactants}^{v_{reactants}} - \frac{1}{K_{eq}} \prod C_{products}^{v_{products}} \right)$$

$$\text{The kinetic constants are based on Arrhenius law : } k = k^{\circ} * \exp \left[-\frac{E_a}{R} \left(\frac{1}{T_{ref}} - \frac{1}{T} \right) \right]$$

With the temperature of reference $T_{ref} = 340^{\circ}\text{C}$

- Aldol reaction rate
- Jones MPV reaction rate
- Jones dehydration rate
- Inoue aldol + intra-MPV reaction rate
- Inoue MPV reaction rate
- Inoue dehydration rate



$$\left(\frac{r_{aldol\ reaction}}{r_{aldol\ reaction+intraMPV}} \right)_{max} = 3.7$$

$$\left(\frac{r_{aldol\ reaction}}{r_{aldol\ reaction+intraMPV}} \right)_{max} = 3.5$$

$$\left(\frac{r_{aldol\ reaction}}{r_{aldol\ reaction+intraMPV}} \right)_{min} = 2.0$$

$$\left(\frac{r_{aldol\ reaction}}{r_{aldol\ reaction+intraMPV}} \right)_{min} = 1.5$$

$$BD\ production_{Inoue} = \frac{r_{aldol\ reaction+intraMPV}}{r_{aldol\ reaction+intraMPV} + r_{aldol\ reaction}}$$