

Primary compounds: $2 \square \square$ VOC_2 $2 \square \square$

Gaseous stack: VOC_n VOC_2 VOC_1

Solubility check
→ $H_{eff} \square \square \square$
→ $H \square \square \square \square \square$

Gas phase protocol
→ $G \square \square \square \square \square \square \square$
 $H \square \square \square \square \square$

$1 \square \square \square \square \square \square \square \square \square \square$

Aqueous stack: $2 \square \square$ $2 \square \square$ $2 \square \square$

Formation of peroxy radicals
→ $\square \square CO_2$

Formation of peroxy radicals with hydroxyl function in -position
→ $\square \square C(OH)O_2$

Formation of peroxy radicals with carboxyl function in -position
→ $\square \square C(O_2)C(=O)OH / \square \square C(O_2)C(=O)O^-$

Formation of oxy radicals
→ $\square \square CO^\bullet$

Formation of acylperoxy radicals
→ $\square \square -C(=O)O^\bullet$

Hydration
 $\square \square C=O \rightleftharpoons \square \square C(OH)_2$

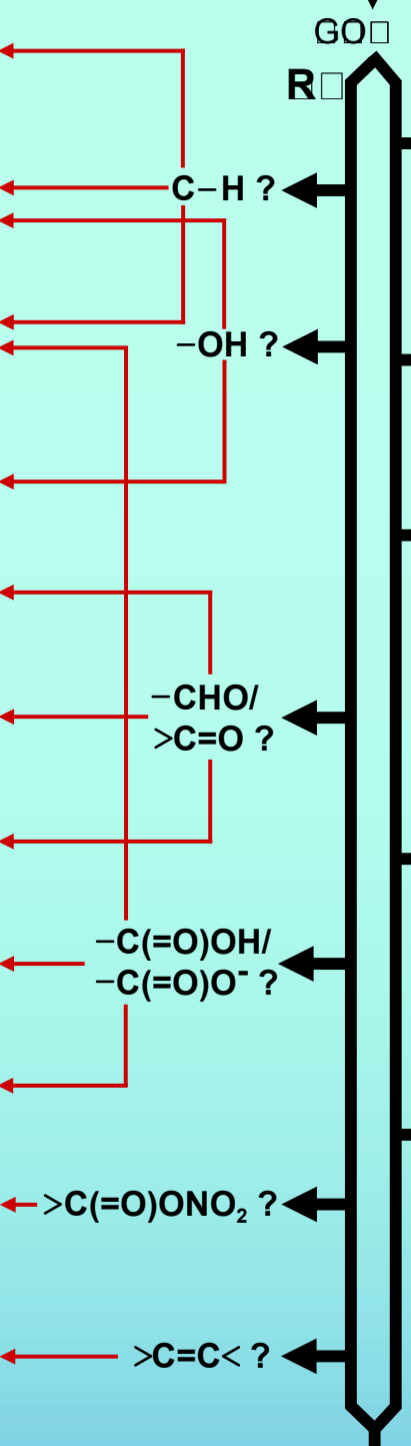
Bond breaking of multi-carbonyls
→ $\square \square CO_2$

Formation of acyloxy radicals
→ $\square \square -C(=O)O^\bullet$

Dissociation
 $\square \square -COOH \rightleftharpoons \square \square -COO^-$

Hydrolysis
 $\square \square C(=O)NO_3 \rightarrow \square \square C(=O)OH + H^+ + NO_3^-$

OH/NO₃ addition to double bond
→ $\square \square \square \square$



Alkoxy chemistry
 $\square \square \square \square \rightarrow \square \square \square$
 $\square \square \square \square \rightarrow \square \square C=O + \square \square C''O_2$

Acyloxy chemistry
 $\square \square -C(=O)O^\bullet + O_2 \rightarrow \square \square \square \square$

Peroxy recombinations and cross reactions
 $\square \square CHO_2^\bullet + \square \square CHO_2^\bullet \rightarrow \square \square -CHO + \square \square CHOH + O_2$
 $\rightarrow \square \square 2 \square \square CHO^\bullet + O_2$
 $\rightarrow \square \square 2 \square \square -CHO + H_2O_2$
 $\square \square CO_2^\bullet + \square \square CO_2^\bullet \rightarrow \square \square 2 \square \square CO^\bullet + O_2$

Special peroxy chemistry
 $\square \square C(OH)O_2 \rightarrow \square \square -CHO + \square \square HO_2$
 $\square \square 2 \square \square C(O_2)C(=O)OH (2 \square \square C(O_2)C(=O)O^- + 2 H_2O)$
 $\rightarrow \square \square 2 \square \square -CHO + 2 \square \square CO_2 + 2 \square \square H_2O_2 (+ 2 \square \square OH^\bullet)$

Acyl peroxy chemistry
 $\square \square \square \square \rightarrow \square \square \square \square$

Solubility check
→ $H_{eff} \square \square \square$
→ $H \square \square \square \square \square$

Check for experimental data
→ Assign experimental rate constant from kinetic database when available

HDFN VOC_n VOC_2 VOC_1

$\square \square \square \square \square \square \square \square$