CRECK Model, 2003 Release (March 2020)

http://creckmodeling.chem.polimi.it/menu-kinetics/menu-kinetics-detailed-mechanisms

Nomenclature

HT = high-temperature mechanism

LT = low-temperature mechanism

NOX = sub-module for nitrogen-oxides

Soot = sub-module for soot particles (based on the Discrete Sectional model)

	Mech Name	#Species	#Reactions		Mech Name	#Species	#Reactions
1	C1_C3_HT	114	1999	10	TOT_HT_LT	492	17790
2	C1_C3_HT_NOx	159	2459	11	TOT_HT_LT_SOOT	576	27369
3	TOT_HT_SOOT	452	24041	12	TOT_HT_LT_SOOT_NOx	621	27829
4	TOT_HT_SOOT_NOx	497	24501	13	TOT_HT_LT_NOx	537	18250
5	TPRF_HT_ALC	254	7568	14	TOT_HT_NOx	413	14922
6	TPRF_HT_LT_ALC	339	9781	15	TOT_HT_ME	402	16118
7	TPRF_HT_ALC_NOx	299	8028	16	TOT_HT_LT_ME	582	21174
8	TOT_HT	368	14462	17	TPRF_HT_LT_ALC_ETHERS	356	10171
9	SYNGAS	21	62	@	Contact us for ad hoc mechanism!		

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Fuel component	Real Fuel	HT	HT+LT	HT +NOx	HT+LT +NOx	HT+SOOT	HT+LT +SOOT	HT+LT +NOx+SOOT	HT +NOx+SOOT
H_2	Syngas	9		2		3			4
CO	Syngas	9		2		3			4
CH_4	Natural gas	1		2		3			4
C_2H_4	Natural gas	1		2		3			4
C_2H_6	Natural gas	1		2		3			4
C_3H_6	Natural gas/LPG	1		2		3			4
C_3H_8	Natural gas/LPG	1		2		3			4
nC_4H_{10}	Natural gas/LPG	1		2		3			4
nC_5H_{12}	LPG	5	6	7	13	3	11	12	4
nC_7H_{16}	Gasoline	5	6	7	13	3	11	12	4
$nC_{10}H_{22}$	Diesel/JetFuel	8	10	14	13	3	11	12	4
$nC_{12}H_{26}$	Diesel/JetFuel	8	10	14	13	3	11	12	4
$nC_{16}H_{34}$	Diesel	8	10	14	13	3	11	12	4
iC_4H_{10}	Natural gas/LPG	1	6	2	13	3	11	12	4
iC_8H_{18}	Gasoline	5	6	7	13	3	11	12	4
$iC_{12}H_{26}$	Diesel/JetFuel	8	10	14	13	3	11	12	4
$iC_{16}H_{34}$	Diesel/JetFuel	8	10	14	13	3	11	12	4
C_6H_6		8	10	14	13	3	11	12	4
$C_6H_5CH_3$	Gasoline	8	10	14	13	3	11	12	4
Xylene	Diesel/JetFuel	8	10	14	13	3	11	12	4
n-propyl-benzene	Diesel/JetFuel	8	10	14	13	3	11	12	4
Tri-methyl-benzene	Diesel/JetFuel	8	10	14	13	3	11	12	4
Cyclo-hexane	Gasoline/JetFuel	8	10	14	13	3	11	12	4

Fuel component	Real Fuel	HT	HT+LT	HT +NOx	HT+LT +NOx	HT+SOOT	HT+LT +SOOT	HT+LT +NOx+SOOT	HT +NOx+SOOT
Methyl-cyclo-hexane	Gasoline/JetFuel	8	10	14	13	3	11	12	4
Decalin	JetFuel	8	10	14	13	3	11	12	4
Methyl-Naphtalene	Diesel/JetFuel	8	10	14	13	3	11	12	4
Methyl-butanoate	Biodiesel	15	16	@	@	@	@	@	@
Methyl-decanoate	Biodiesel	15	16	@	@	@	@	@	@
Methyl-palmitate	Biodiesel	15	16	@	@	@	@	@	@
Methyl-stearate	Biodiesel	15	16	@	@	@	@	@	@
Methyl-linoleate	Biodiesel	15	16	@	@	@	@	@	@
Methyl-linolenate	Biodiesel	15	16	@	@	@	@	@	@
Phenol	Bio-oil	8	10	14	13	3	11	12	4
Anisole	Bio-oil	8	10	14	13	3	11	12	4
Guaiacol	Bio-oil	8	10	14	13	3	11	12	4
Catechol	Bio-oil	8	10	14	13	3	11	12	4
Vanillin	Bio-oil	8	10	14	13	3	11	12	4
Acetic Acid	Bio-oil	5	6	7	13	3	11	12	4
Butanoic Acid	Bio-oil	@	@	@	@	@	@	@	@
Pentanoic Acid	Bio-oil	@	@	@	@	@	@	@	@
Ethanol	Biogasoline	5	6	7	13	3	11	12	4
i-propanol	Biofuel	5		14		3			4
n-propanol	Biofuel	5	6	14	13	3	11	12	4
n-butanol	Biofuel/Bio-oil	5	6	14	13	3	11	12	4
n-pentanol	Biofuel/Bio-oil	5	6	14	13	3	11	12	4
n-hexanol	Biofuel/Bio-oil	5	6	14	13	3	11	12	4

Fuel component	Real Fuel	HT	HT+LT	HT +NOx	HT+LT +NOx	HT+SOOT	HT+LT +SOOT	HT+LT +NOx+SOOT	HT +NOx+SOOT
Iso-butanol	Biofuel	5	NA	14	NA	3	NA	NA	4
ter-butanol	Biofuel	5	NA	14	NA	3	NA	NA	4
2-butanol	Biofuel	5	NA	14	NA	3	NA	NA	4
Iso-pentanol	Biofuel	5	NA	14	NA	3	NA	NA	4
Propanal	Bio-oil	5	6	14	13	3	11	12	4
n-butanal	Bio-oil	5	6	14	13	3	11	12	4
n-pentanal	Bio-oil	5	6	14	13	3	11	12	4
n-hexanal	Bio-oil	5	6	14	13	3	11	12	4
Iso-butanal	Bio-oil	5	6	14	13	3	11	12	4
DME	Gasoline	17	17	@	@	@	@	@	@
MTBE	Gasoline	17	17	@	@	@	@	@	@
DIPE	Gasoline	17	17	@	@	@	@	@	@
TAME	Gasoline	17	17	@	@	@	@	@	@
ETBE	Gasoline	17	17	@	@	@	@	@	@