

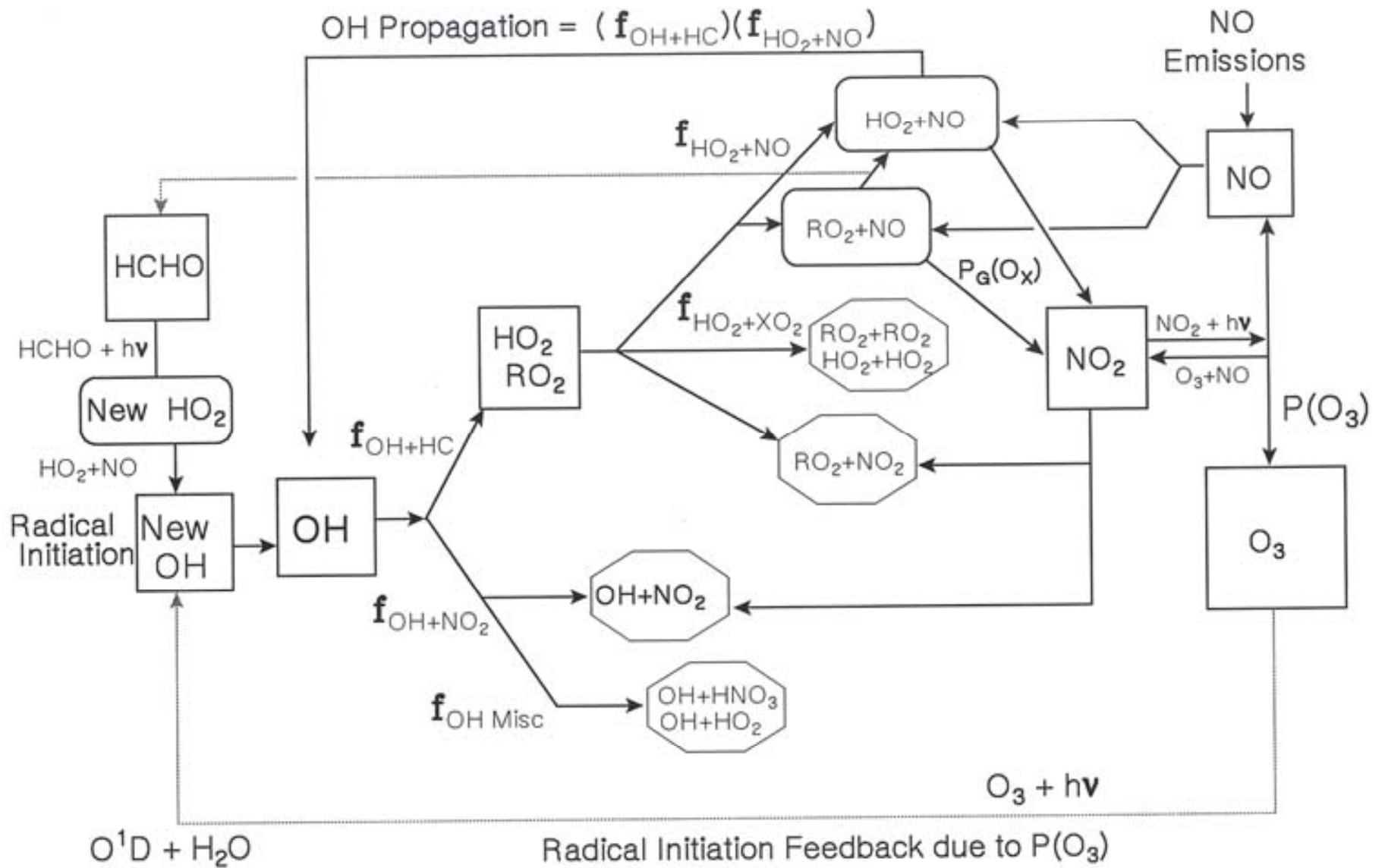
Atmospheric Chemical Mechanisms: Tackling the Greatest Uncertainties

Trip report for conference at U. California-Davis,
December 2010

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TCEQ Air Modeling and Data Analysis Section

February 24, 2011

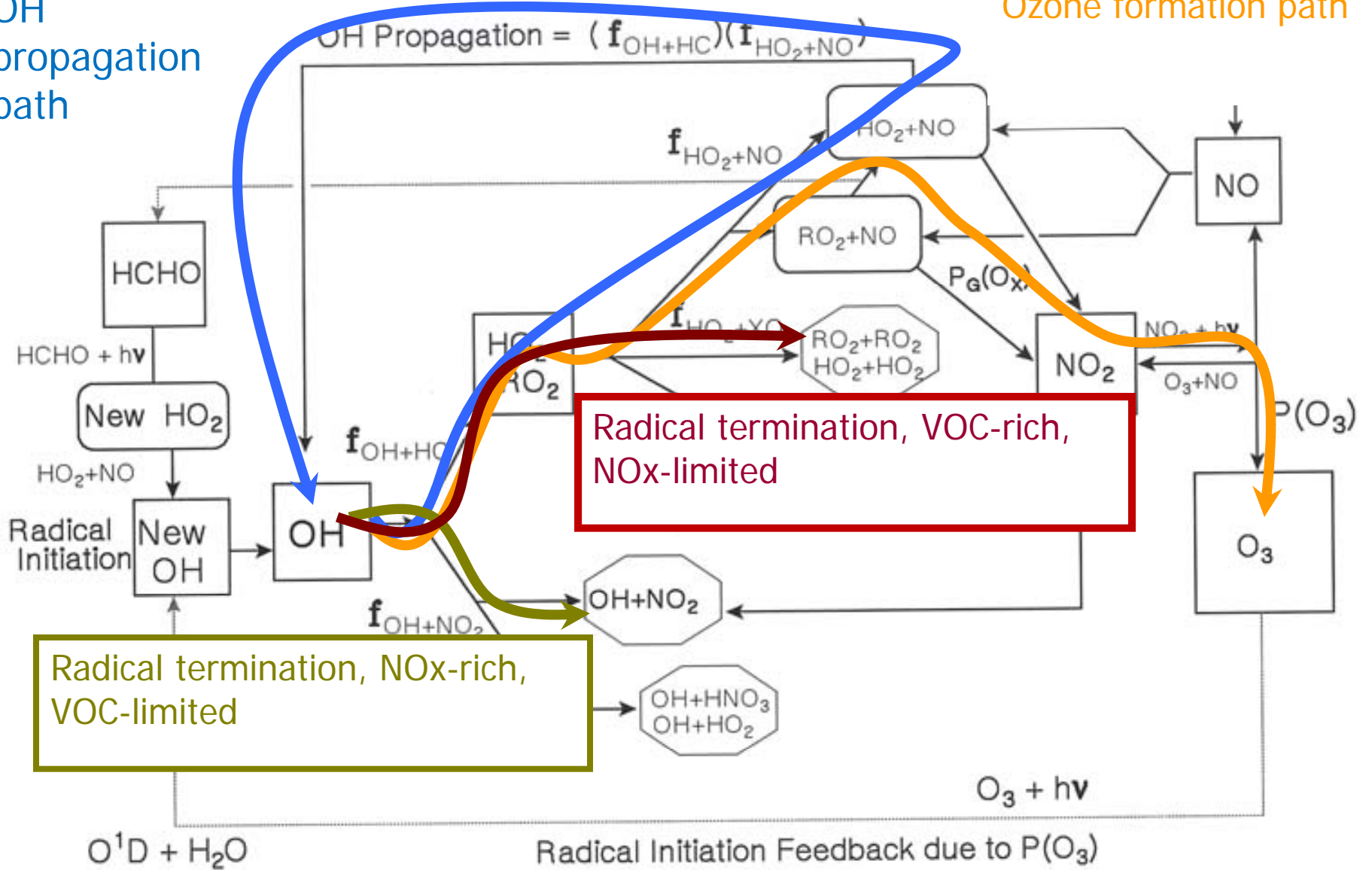


STOP sign indicates radical termination

From Tonnesen, UC-Riverside

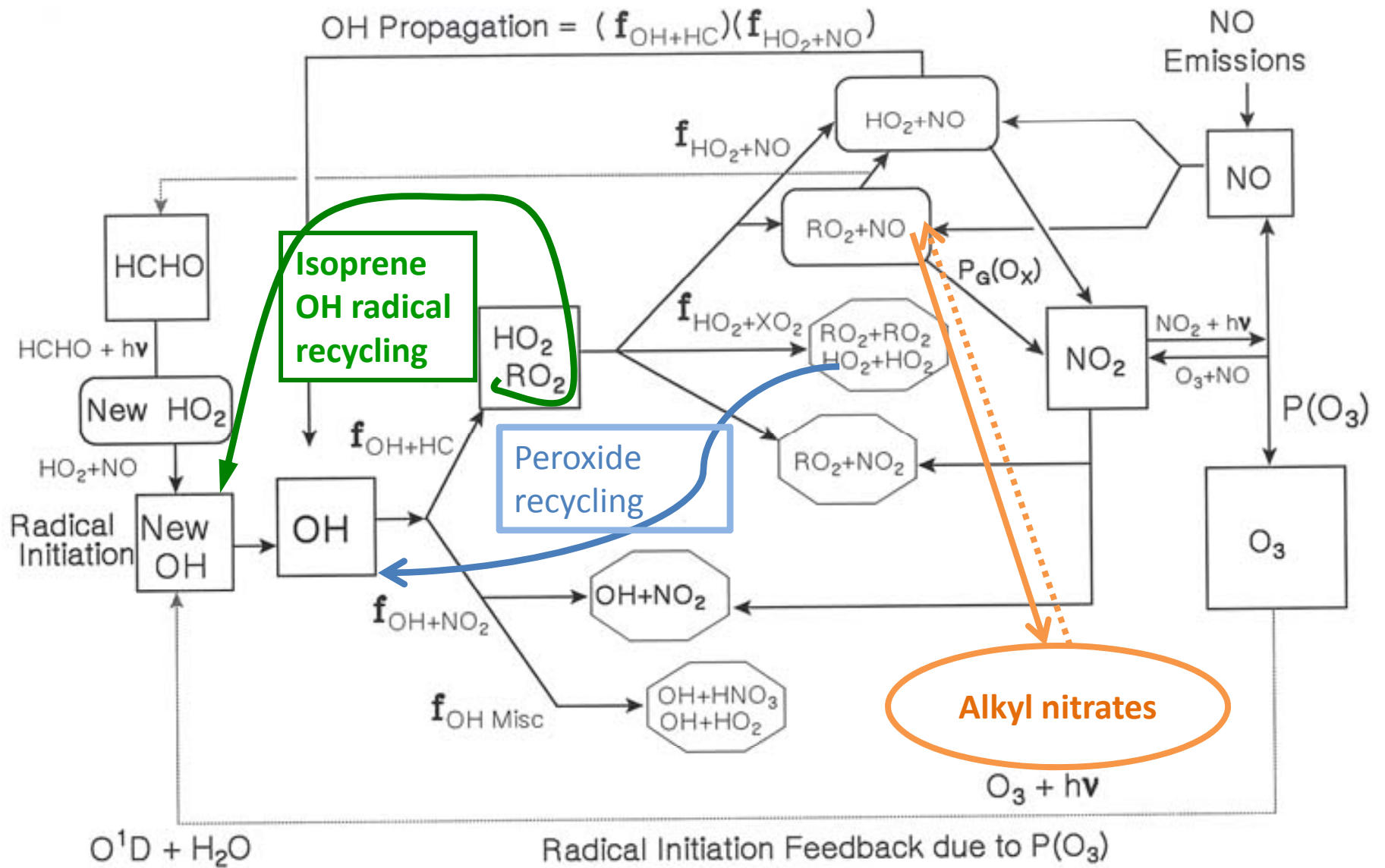
OH propagation path

Ozone formation path

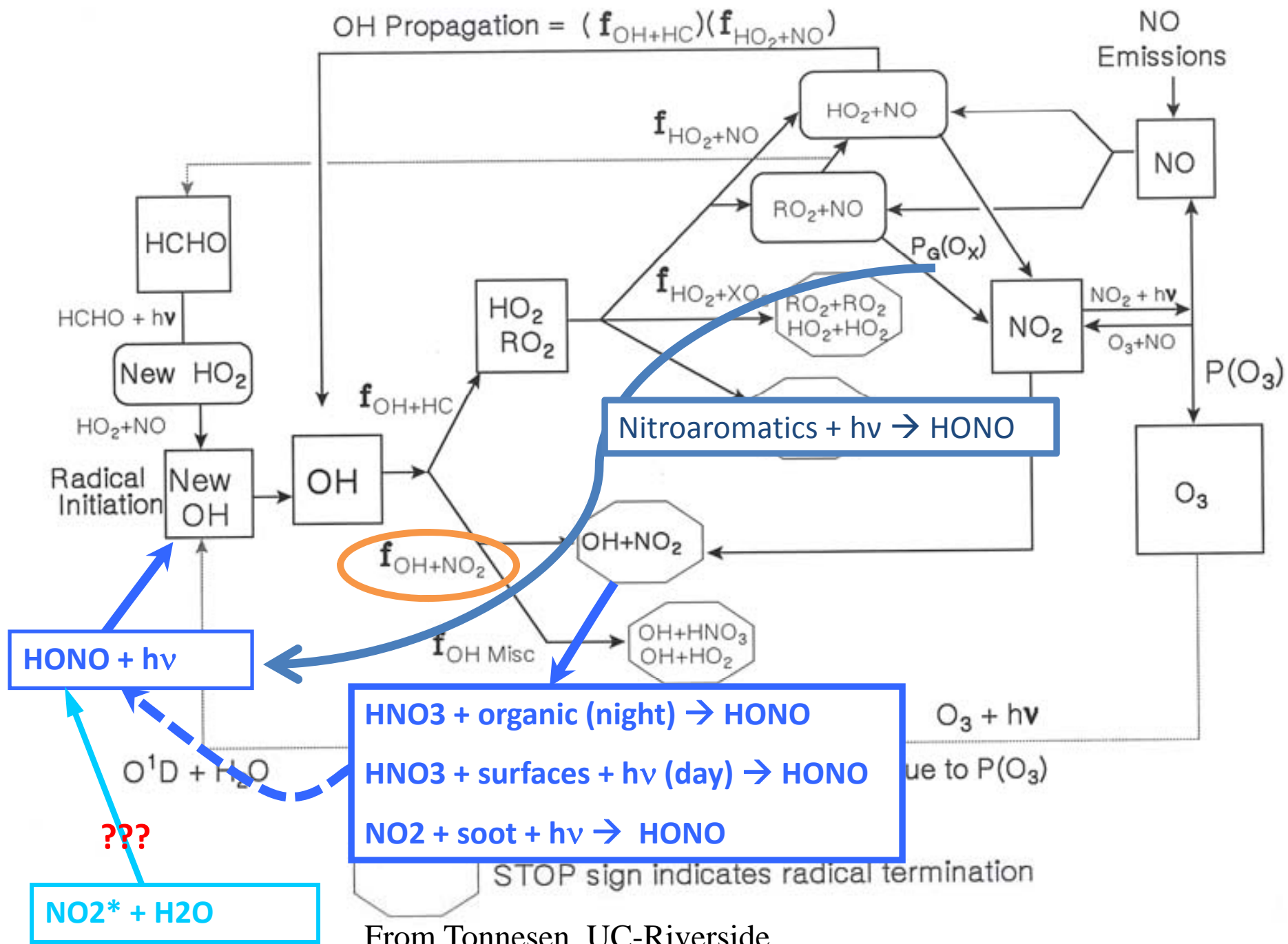


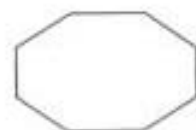
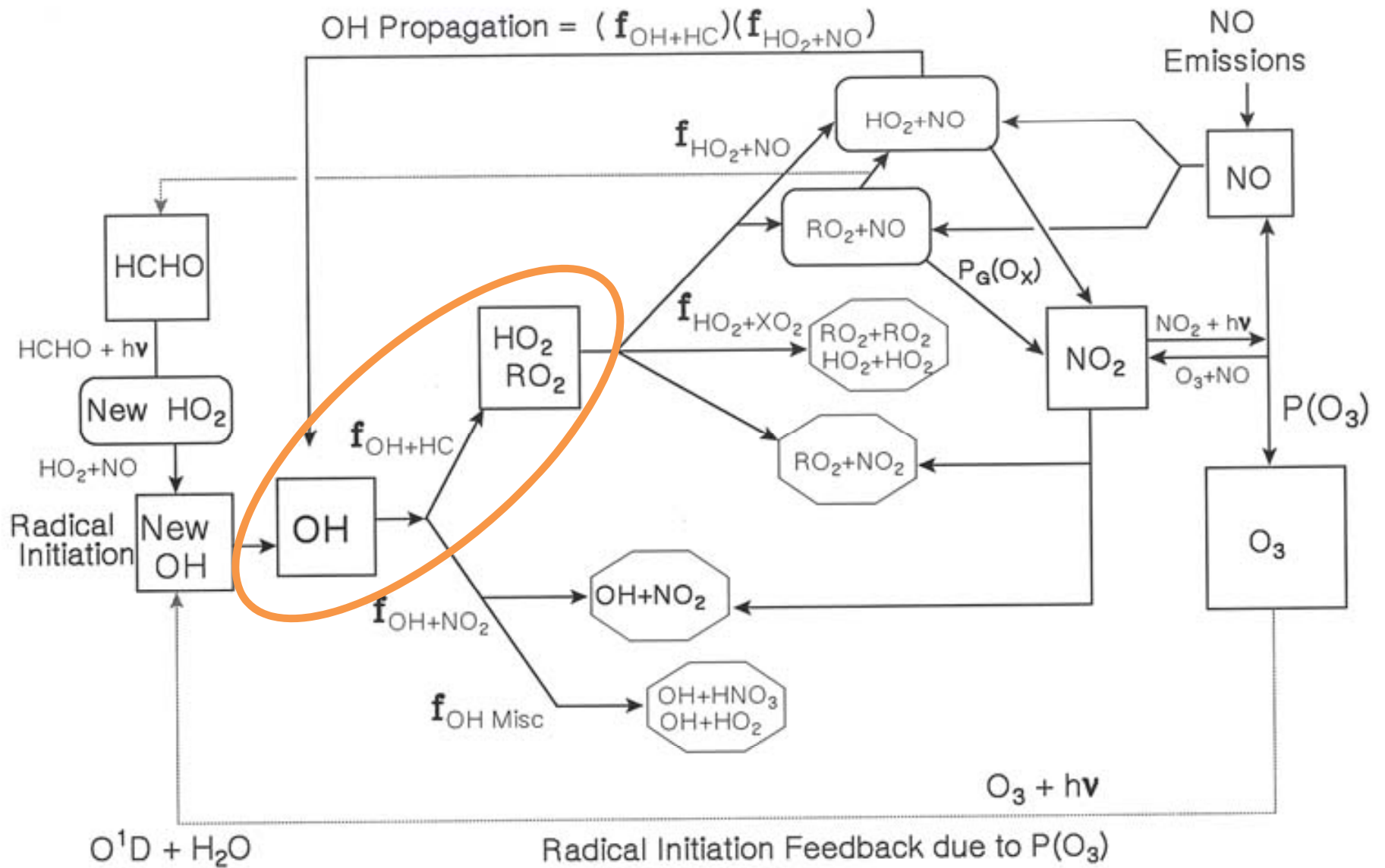
 STOP sign indicates radical termination

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STOP sign indicates radical termination

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a. The simplified form:

OH + hydrocarbon (e.g., isoprene)
→ HO₂, RO₂

149:	ISOP + OH = ISO2 + RO2	163:	EPX2 + HO2 = 0.275 GLYD + 0.275 GLY + 0.275MGLY + 1.125 OH + 0.825 HO2 + 0.375 FORM + 0.074 FACD + 0.251 CO + 2.175 PAR
150 :	ISO2 + NO = 0.117 INTR + 0.883 NO2 + 0.803 HO2 + 0.66 FORM + 0.66 ISPD + 0.08 XO2H + 0.08 RO2 + 0.05 IOLE + 0.042 GLYD + 0.115 PAR + 0.038 GLY + 0.042 MGLY + 0.093 OLE + 0.117 ALDX	164:	EPX2 + NO = 0.275 GLYD + 0.275 GLY + 0.275MGLY + 0.125 OH + 0.825 HO2 + 0.375 FORM + NO2 + 0.251 CO + 2.175 PAR
151:	ISO2 + HO2 = 0.88 ISPX + 0.12 OH + 0.12 HO2 + 0.12 FORM + 0.12 ISPD	165:	EPX2 + C2O3 = 0.22 GLYD + 0.22 GLY + 0.22 MGLY + 0.1 OH + 0.66 HO2 + 0.3 FORM + 0.2 CO + 1.74PAR + 0.8 MEO2 + 0.2 AACD + 0.8 RO2
152:	ISO2 + C2O3 = 0.709 HO2 + 0.583 FORM + 0.583 ISPD + 0.071 XO2H + 0.044 IOLE + 0.037 GLYD + 0.102 PAR + 0.034 GLY + 0.037 MGLY + 0.082 OLE + 0.103 ALDX + 0.8 MEO2 + 0.2 AACD + 0.871 RO2	166:	EPX2 + RO2 = 0.275 GLYD + 0.275 GLY + 0.275MGLY + 0.125 OH + 0.825 HO2 + 0.375 FORM + 0.251 CO + 2.175 PAR + RO2
153:	ISO2 + RO2 = 0.803 HO2 + 0.66 FORM + 0.66 ISPD + 0.08 XO2H + 0.05 IOLE + 0.042 GLYD + 0.115 PAR + 0.038 GLY + 0.042 MGLY + 0.093 OLE + 0.117 ALDX + 1.08 RO2	167 :	INTR + OH = 0.63 XO2 + 0.37 XO2H + RO2 + 0.444NO2 + 0.185 NO3 + 0.104 INTR + 0.592 FORM + 0.331 GLYD + 0.185 FACD + 2.7 PAR + 0.098 OLE + 0.078 ALDX + 0.266 NTR
154:	ISO2 = 0.8 HO2 + 0.04 OH + 0.04 FORM + 0.8 ISPD		
155:	ISOP + O3 = 0.6 FORM + 0.65 ISPD + 0.15 ALDX + 0.2 CXO3 + 0.35 PAR + 0.266 OH + 0.2 XO2 + 0.2RO2 + 0.066 HO2 + 0.066 CO		
156:	ISOP + NO3 = 0.35 NO2 + 0.65 INTR + 0.64 XO2H + 0.33 XO2 + 0.03 XO2N + RO2 + 0.35 FORM + 0.35ISPD		
157:	ISPD + OH = 0.095 XO2N + 0.379 XO2 + 0.318 XO2H + 0.792 RO2 + 0.843 PAR + 0.379 C2O3 + 0.209 CXO3 + 0.379 GLYD + 0.24 MGLY + 0.24 FORM + 0.067 OLE + 0.079 CO + 0.028 ALDX		
158:	ISPD + O3 = 0.02 ALD2 + 0.15 FORM + 0.225 CO + 0.85 MGLY + 0.36 PAR + 0.114 C2O3 + 0.064 XO2H + 0.064 RO2 + 0.268 OH + 0.09 HO2		
159:	ISPD + NO3 = 0.643 CO + 0.282 FORM + 0.357 ALDX + 1.282 PAR + 0.85 HO2 + 0.075 CXO3 + 0.075 XO2H + 0.075 RO2 + 0.85 NTR + 0.15 HNO3		
160:	ISPD + hv = 0.333 CO + 0.067 ALD2 + 0.9 FORM + 0.832PAR + 0.333 HO2 + 0.7 XO2H + 0.7 RO2 + 0.967C2O3		
161:	ISPX + OH = 0.904 EPOX + 0.933 OH + 0.067 ISO2 + 0.067 RO2 + 0.029 IOLE + 0.029 ALDX		
162 :	EPOX + OH = EPX2 + RO2		

c. The Carbon Bond 6 form: condensed from the complex form; more sophisticated than the simple form.