第48回燃焼シンポジウムワークショップ
『ユニバーサル燃焼反応モデルの可能性を探る』

高圧衝撃波管実験による トルエン着火反応モデルの検証

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Introduction

急速圧縮機 (RCM)		衝撃波管 (ST)
ピストン圧縮	⟷	衝撃波加熱
昇温時間が長い	⟷	昇温時間が短い
熱損失が大きい	⟷	熱損失が小さい

1. PRFの包括的詳細反応モデル

	Species	Reactions
Curran (2002)	1034	4236
Ogura (2007)	361	1197

2. トルエン燃焼反応モデル

	Species	Reactions
Pitz (2002)	379	1621
Dagaut (2002)	120	921
Sakai (2007)	299	1570

Validation of Sakai & Dagaut Models

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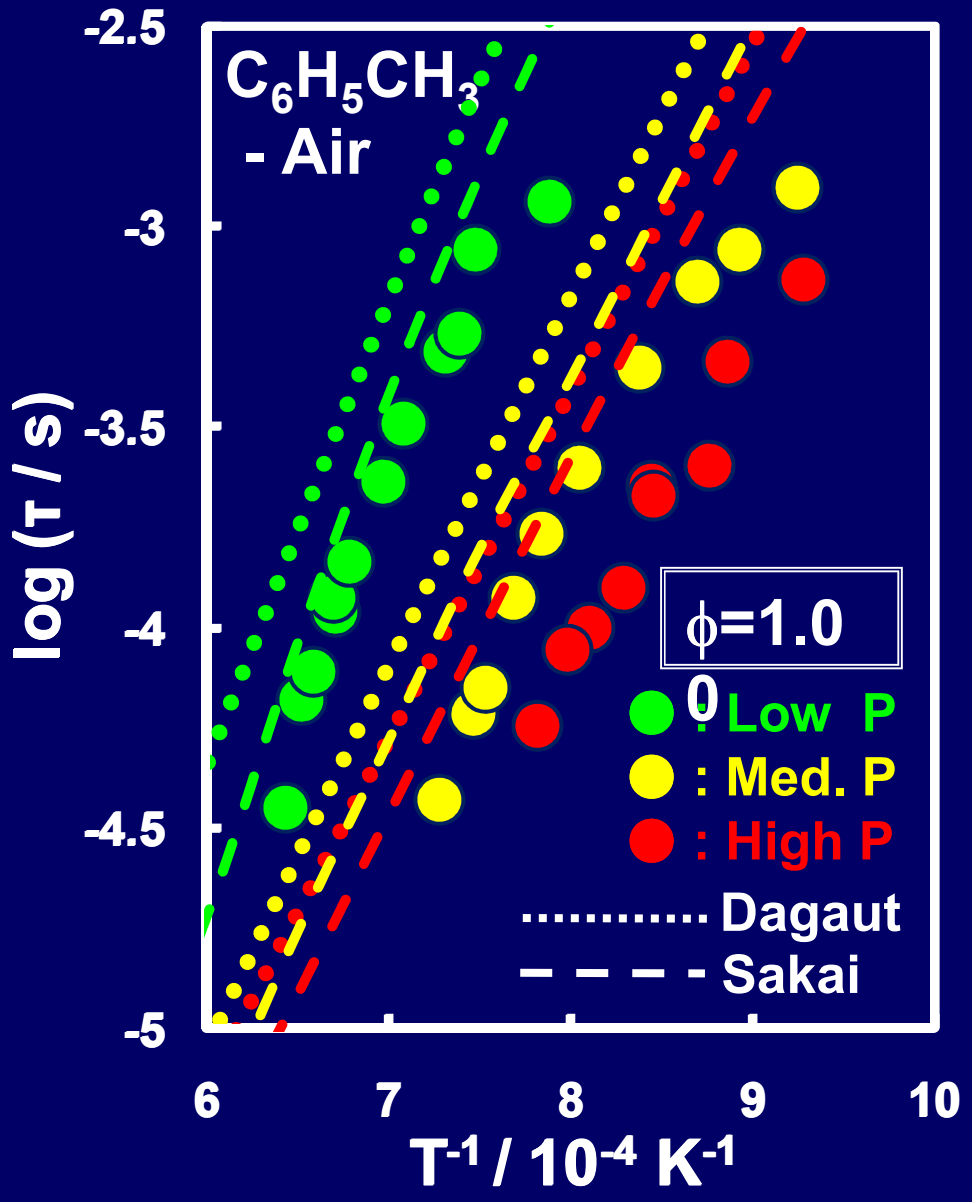
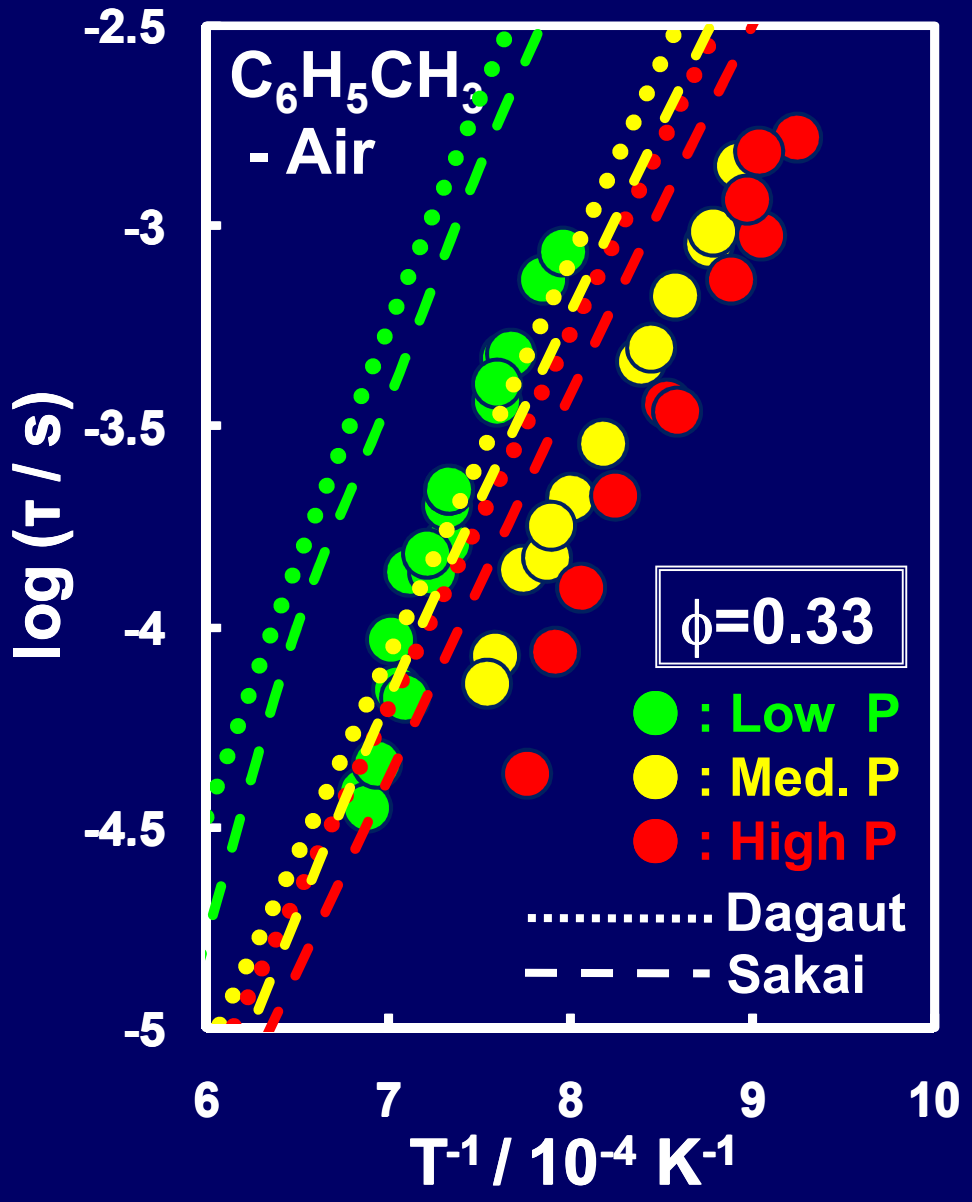


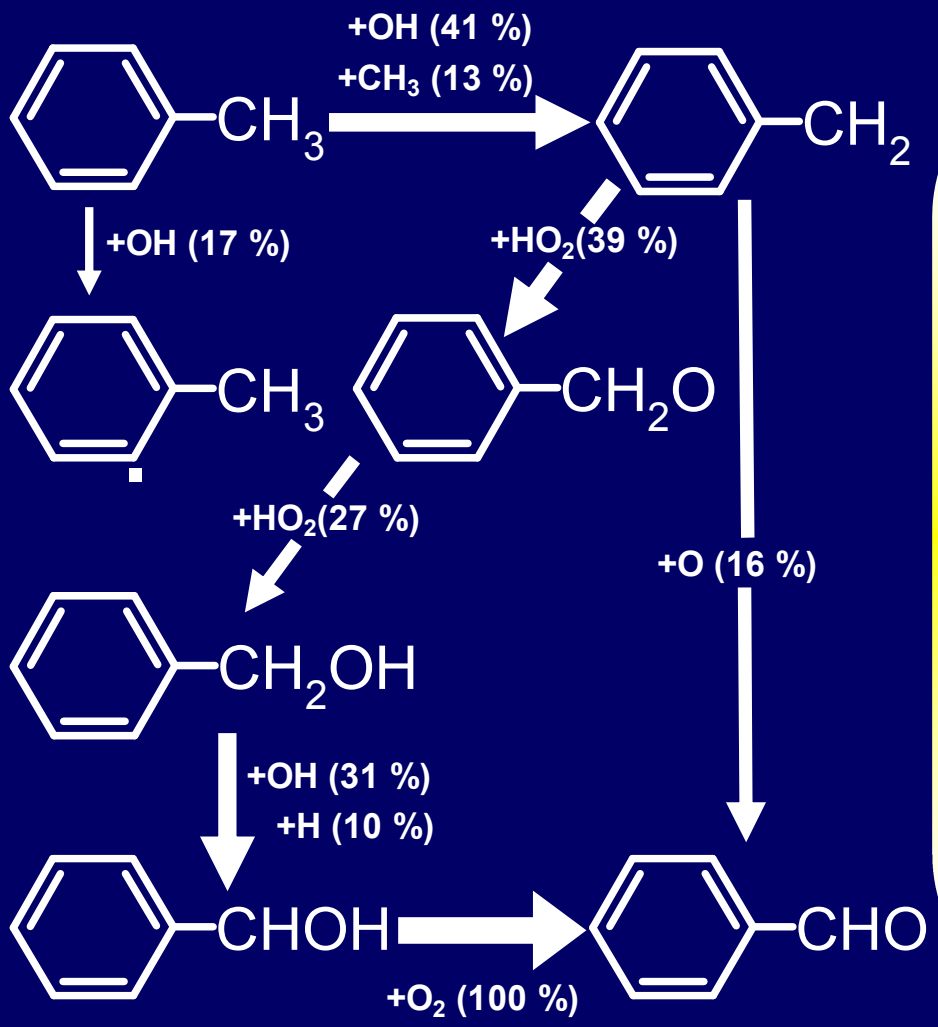


Difference between τ_{exp} and τ_{cal} (Part 1)

$C_6H_5CH_3$ - Air / Model	ϕ = 1.00			ϕ = 0.33		
	2 atm	30 atm	50 atm	2 atm	30 atm	50 atm
Dagaut	139 %	261 %	408 %	472 %	320 %	482 %
Sakai	30 %	115 %	166 %	242 %	143 %	185 %

Green : < 100 %
Aqua : 100 % - 200 %
White : 200 % - 400 %
Pink : 400 % - 900 %
Red : 900 % <

Modification of Sakai Model



1. Reactions of Benzyl Radicals

$C_6H_5CH_2 + HO_2 \rightarrow C_6H_5CH_2O + OH$

$C_6H_5CH_2 + O \rightarrow C_6H_5CHO + H$

$C_6H_5CH_2 + O \rightarrow C_6H_5 + CH_2O$

2. P-dependent Reactions

$C_6H_5CH_3 \rightarrow C_6H_5CH_2 + H$

$C_6H_5CH_3 \rightarrow C_6H_5 + CH_3$

$C_6H_5CH_2O \rightarrow C_6H_5CHO + H$

$C_6H_5CH_2O \rightarrow C_6H_5 + CH_2O$

Validation of the Modified Model

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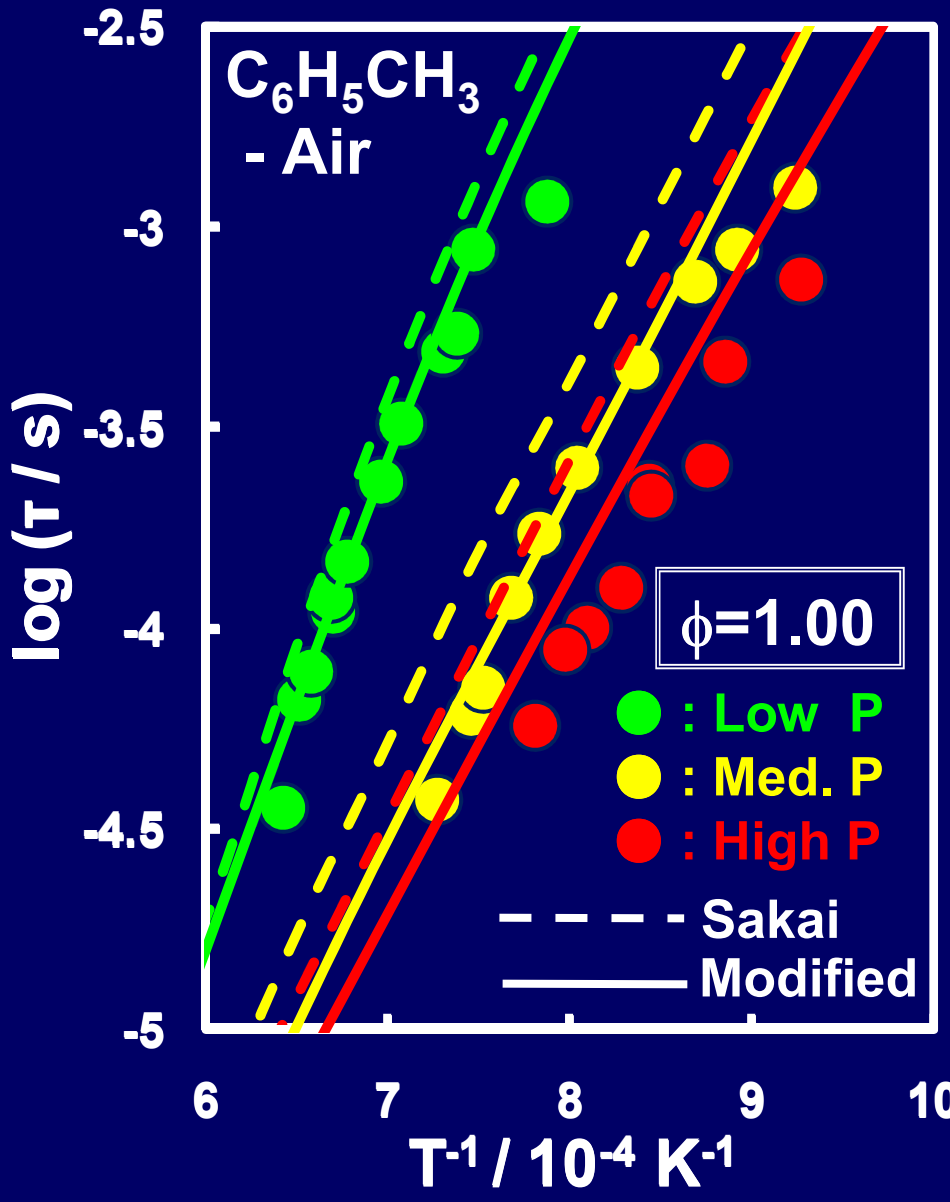

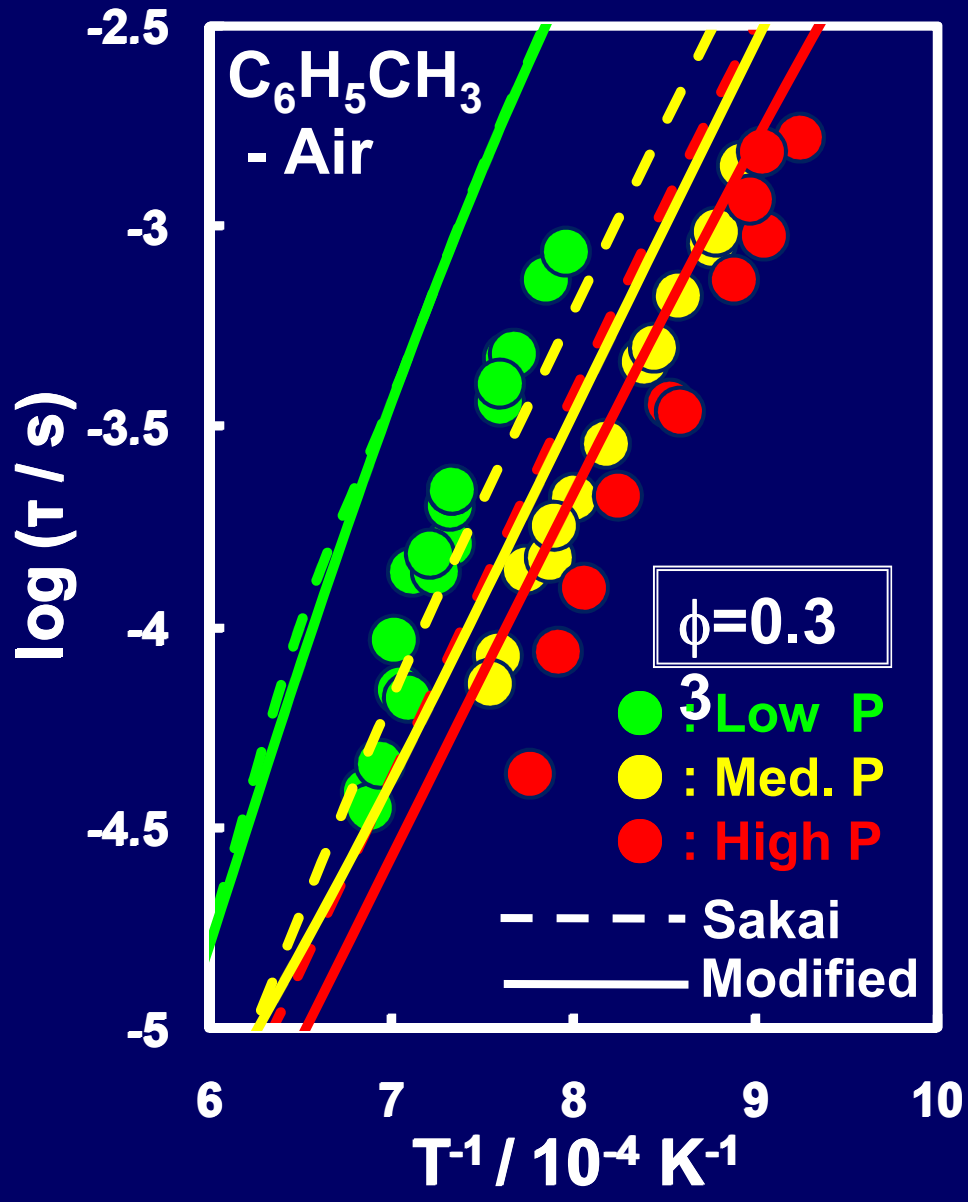

Difference between τ_{exp} and τ_{cal} (Part 2)

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Model \ $C_6H_5CH_3$ - Air	ϕ = 1.00			ϕ = 0.33		
	2 atm	30 atm	50 atm	2 atm	30 atm	50 atm
Sakai	30 %	115 %	166 %	242 %	143 %	185 %
Modified	-16 %	20 %	42 %	242 %	75 %	69 %

Green : < 100 %
Aqua : 100 % - 200 %
White : 200 % - 400 %
Pink : 400 % - 900 %
Red : 900 % <

Reaction Pathway of Toluene Oxidation

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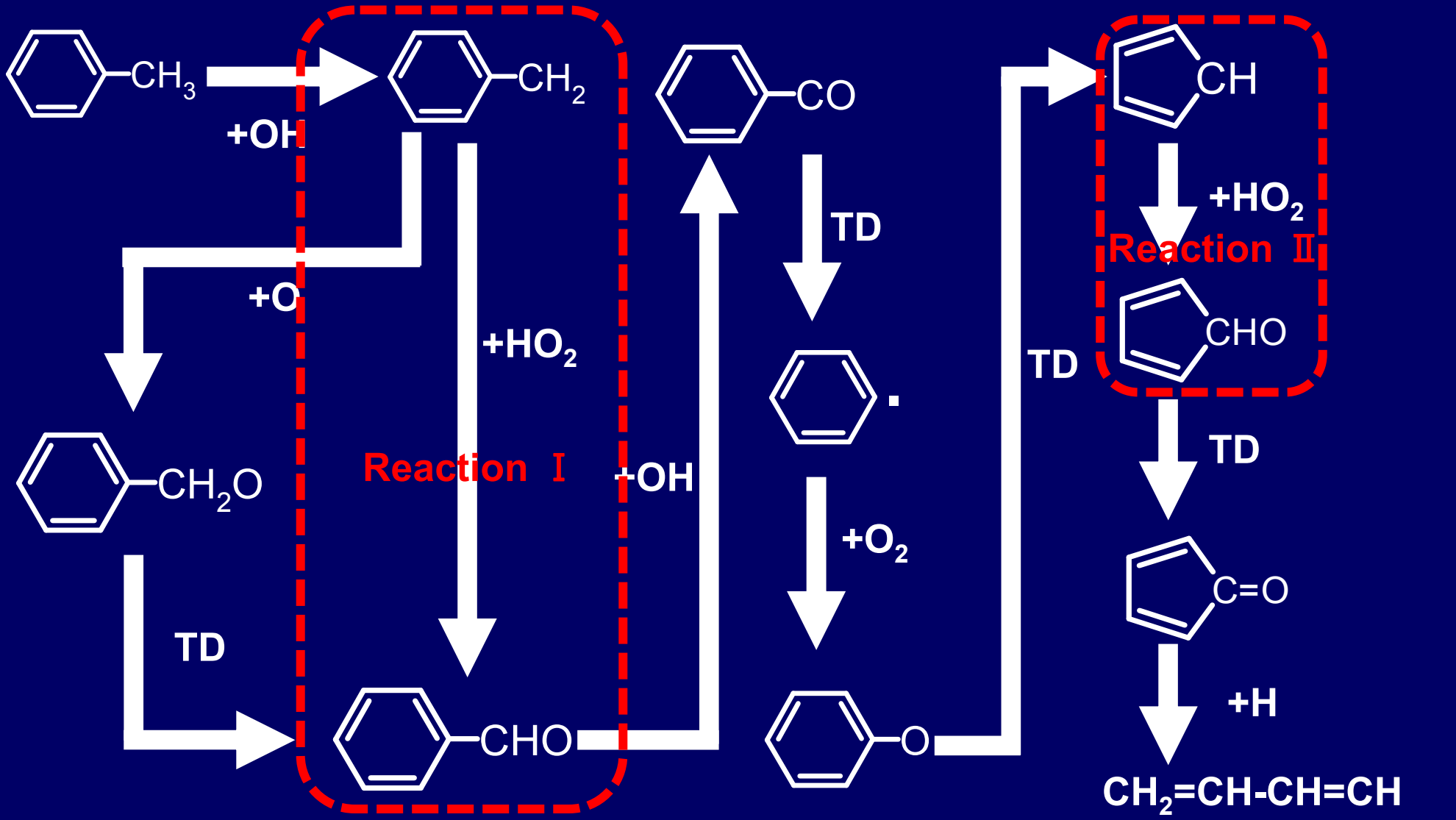

TD: Thermal decomposition

@ 1200K 26.6 atm

Reaction Pathway of Toluene Oxidation

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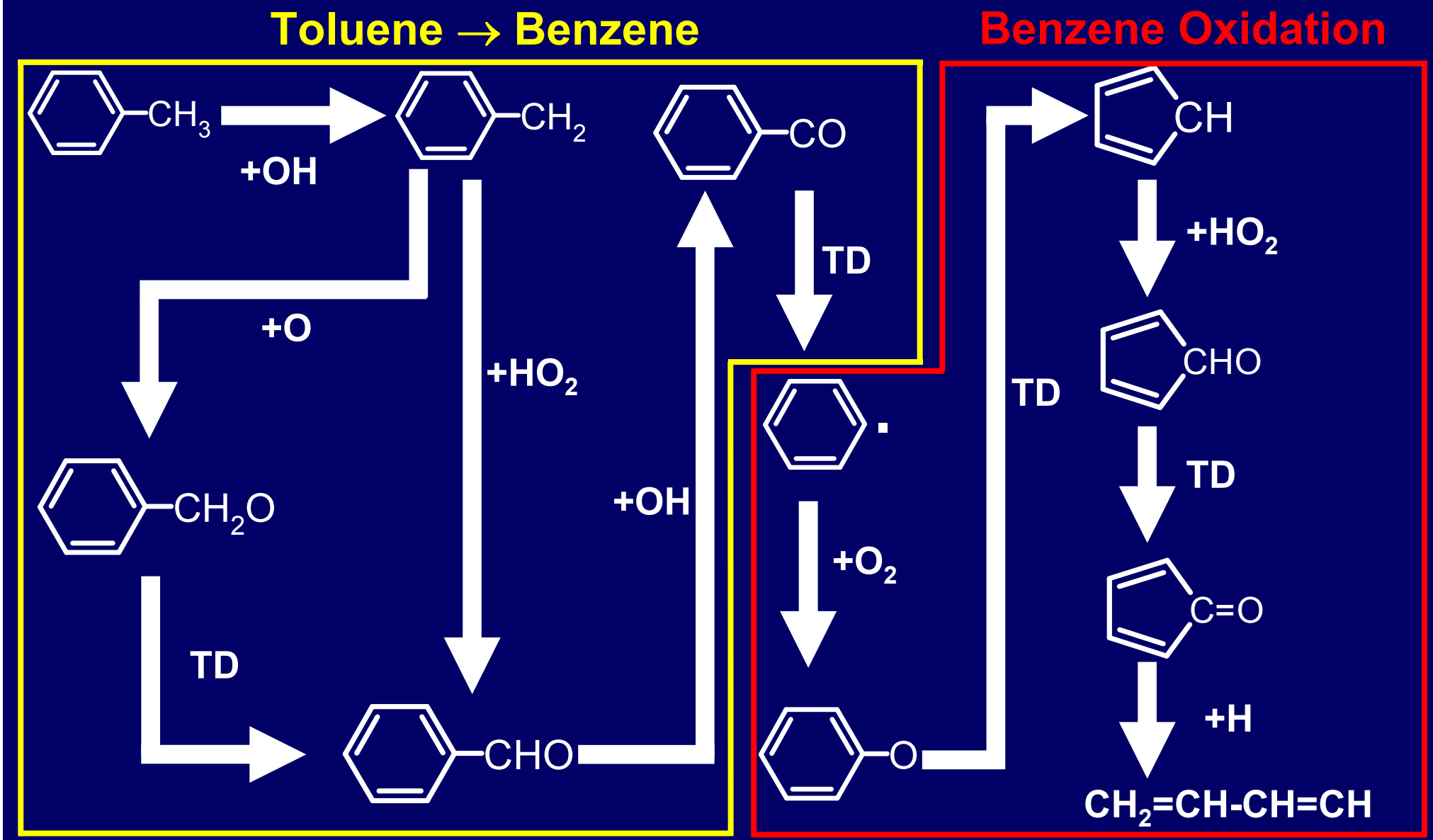

TD: Thermal decomposition

@ 1200K 26.6 atm

Validation of the Models for Benzene Ignitions

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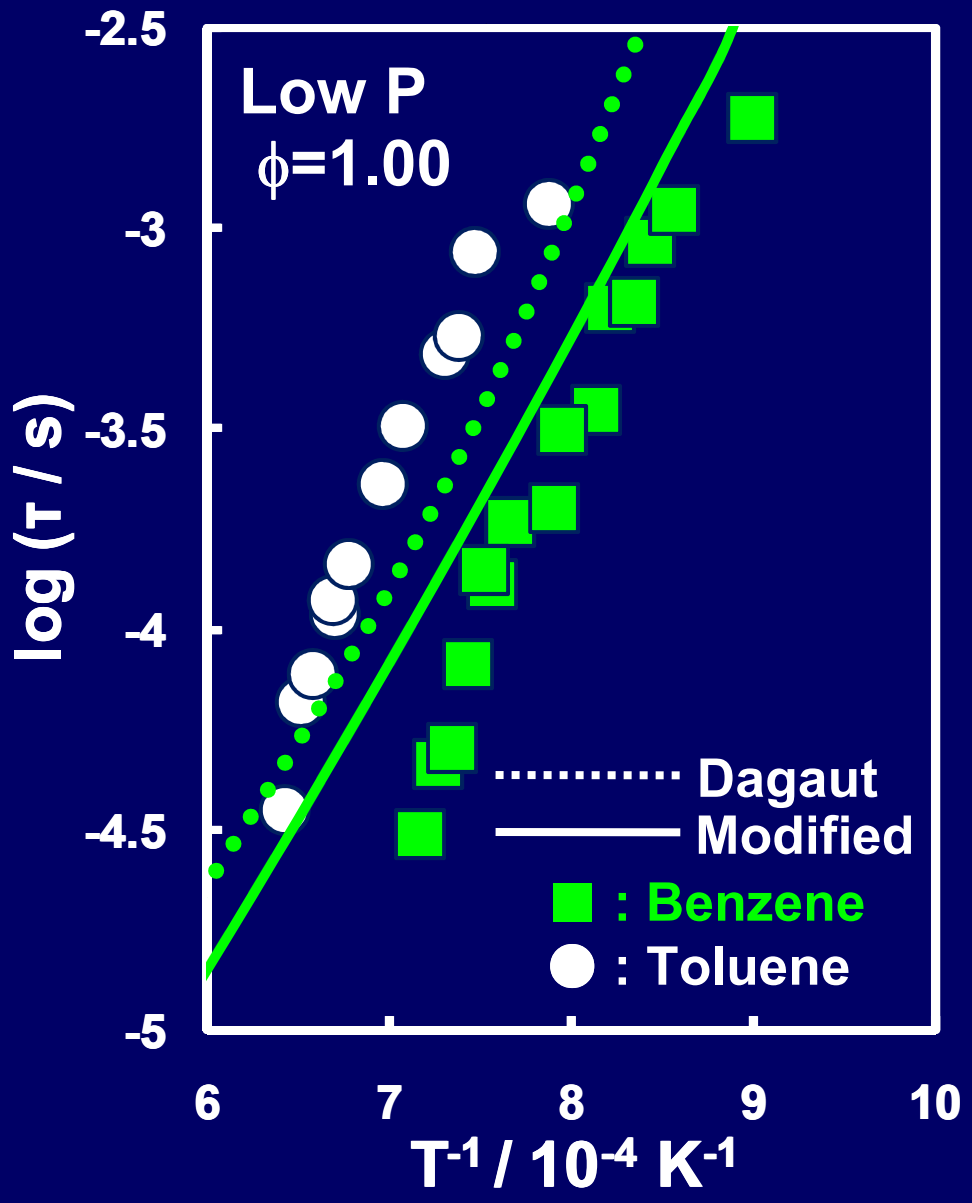

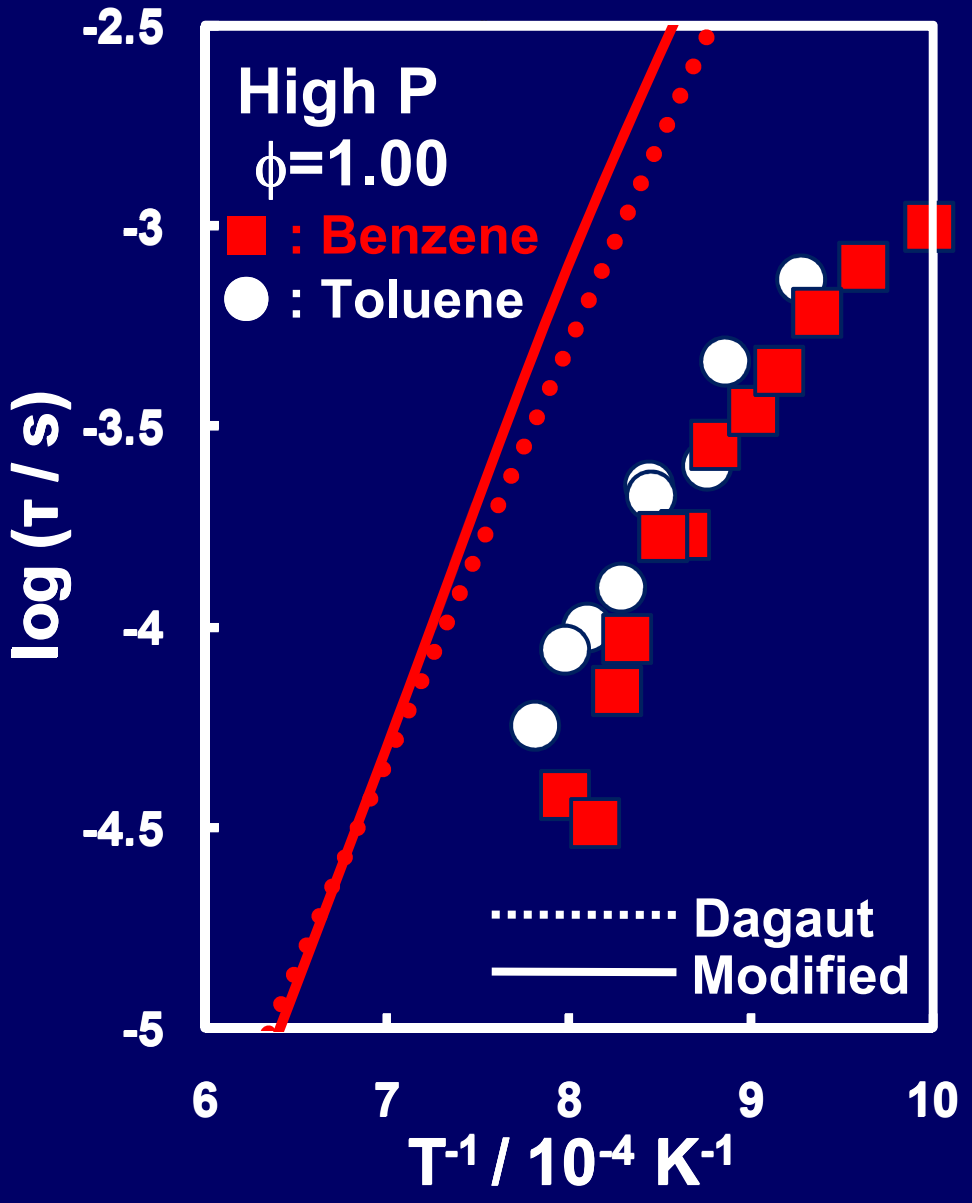

Difference between τ_{exp} and τ_{cal} for Benzene Ignitions

C_6H_6 - Air / Model	ϕ = 1.00	
	2 atm	50 atm
Dagaut	226 %	2031 %
Sakai	109 %	3208 %
Modified	109 %	3208 %

Green : < 100 %
Aqua : 100 % - 200 %
White : 200 % - 400 %
Pink : 400 % - 900 %
Red : 900 % <

Conclusive Remarks

1. τの実測値と計算値(改良モデル)との比較

	ϕ = 1.00			ϕ = 0.33		
	2 atm	30 atm	50 atm	2 atm	30 atm	50 atm
Toluene	-16 %	20 %	42 %	242 %	75 %	69 %
Benzene	109 %	---	3208 %	---	---	---

2. トルエン燃焼反応モデルの課題

- 高圧におけるベンゼン着火遅れ時間を再現できず
  ⇒ ベンゼン燃焼反応モデルの検討が必要
- HO_2との反応の寄与について検討が必要