Explosion Group
TU Delft

SAFEKINEX project

Background and work structure

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- **Dr Kai Holtappels and Dr Volkmar Schröder**

Accidents in process industry

Can an explosion be avoided?

Explosion Indices

Explosion sensitivity: LEL, UEL (FL), LOC, MIE, AIT, CFT, MIT, MESG, LFP, UFP (flash points), ignition delay time (AIT), induction time (CFT) selfheating (smouldering) temp

Explosion severity: P_{max}, $(dP/dt)_{max}$, K_{st}, K_g, flame speed, burning velocity (laminar, turbulent), pressure pulse

Both engineering and chemical factors play a role in these explosion indices

Effects of running conditions on explosion sensitivity indices

Indices related to the explosion sensitivity	**Effect of increased pressure**	**Effect of increased temperature**	**Effect of increased turbulence**
Lower explosion limit (LEL)	Decreases slightly	Decreases	Increases
Upper explosion limit (UEL)	Increases	Increases	Decreases
Lower flash point (LFP)	Increases	not applicable	Increases
Upper flash point (UFP)	Increases	not applicable	Increases
Minimum auto-ignition temperature (AIT)	Decreases	not applicable	Increases
Minimum ignition energy (MIE)	Decreases	Decreases	Increases
Maximum experimental safe gap (MESG)	Decreases	Decreases	Decreases
Limiting oxygen concentration (LOC)	Decreases	Decreases	Increases

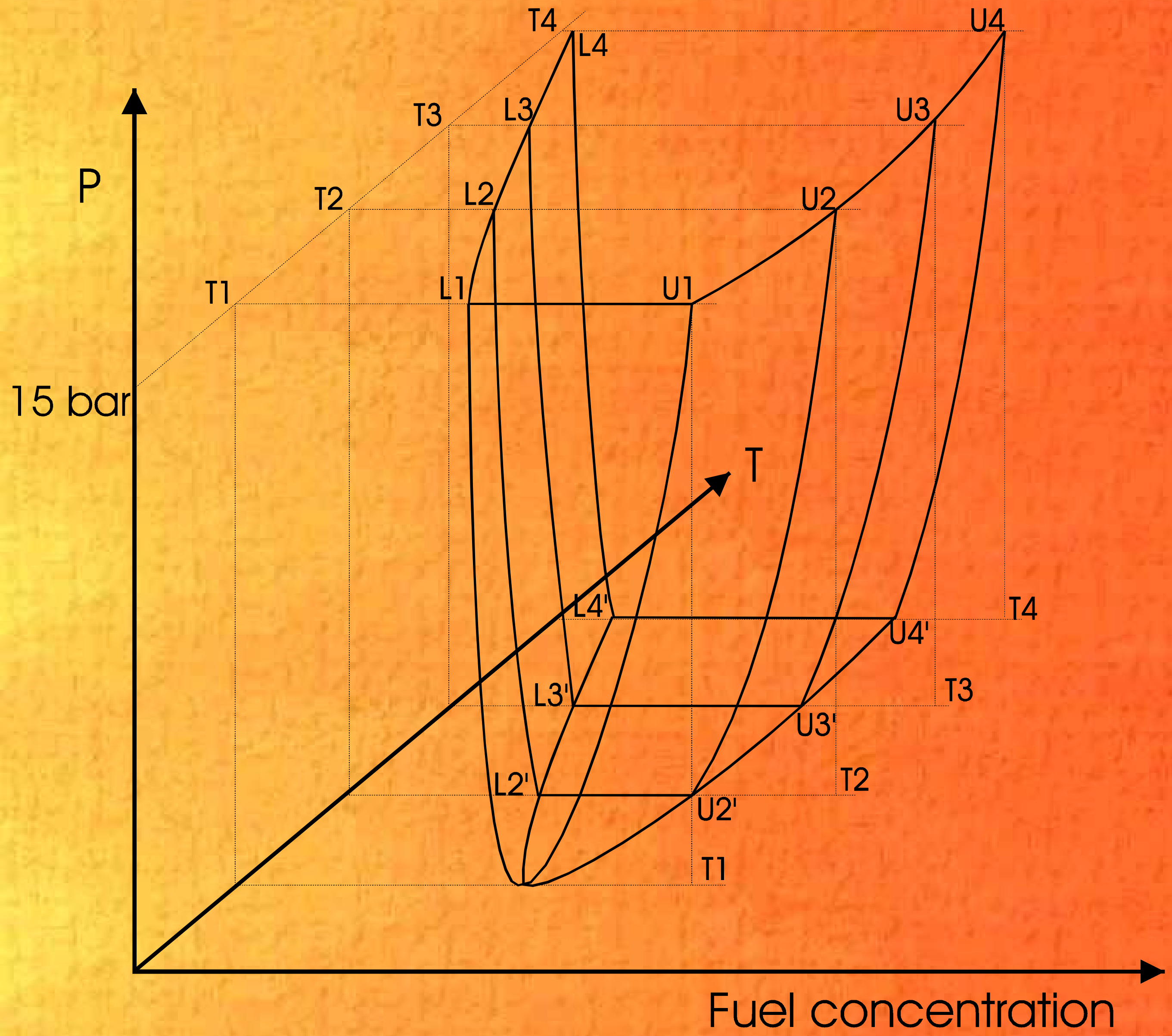
Effects of running conditions on explosion severity indices

Explosion severity term	Effect of increased pressure	Effect of increased temperature	Effect of increased turbulence
Flame speed (S_f)	May slightly decrease or increase	Increases	Increases strongly
P_{max}	Increases linearly	Decreases	May slightly increase
$(dP/dt)_{max}$	Increases linearly	Can increase or decrease	Increases strongly
K-value: (K_G or K_{St})	Increases linearly	Can increase or decrease	Increases strongly

Conclusion:

All explosion indices are affected by changes in pressure, temperature, turbulence, etc.

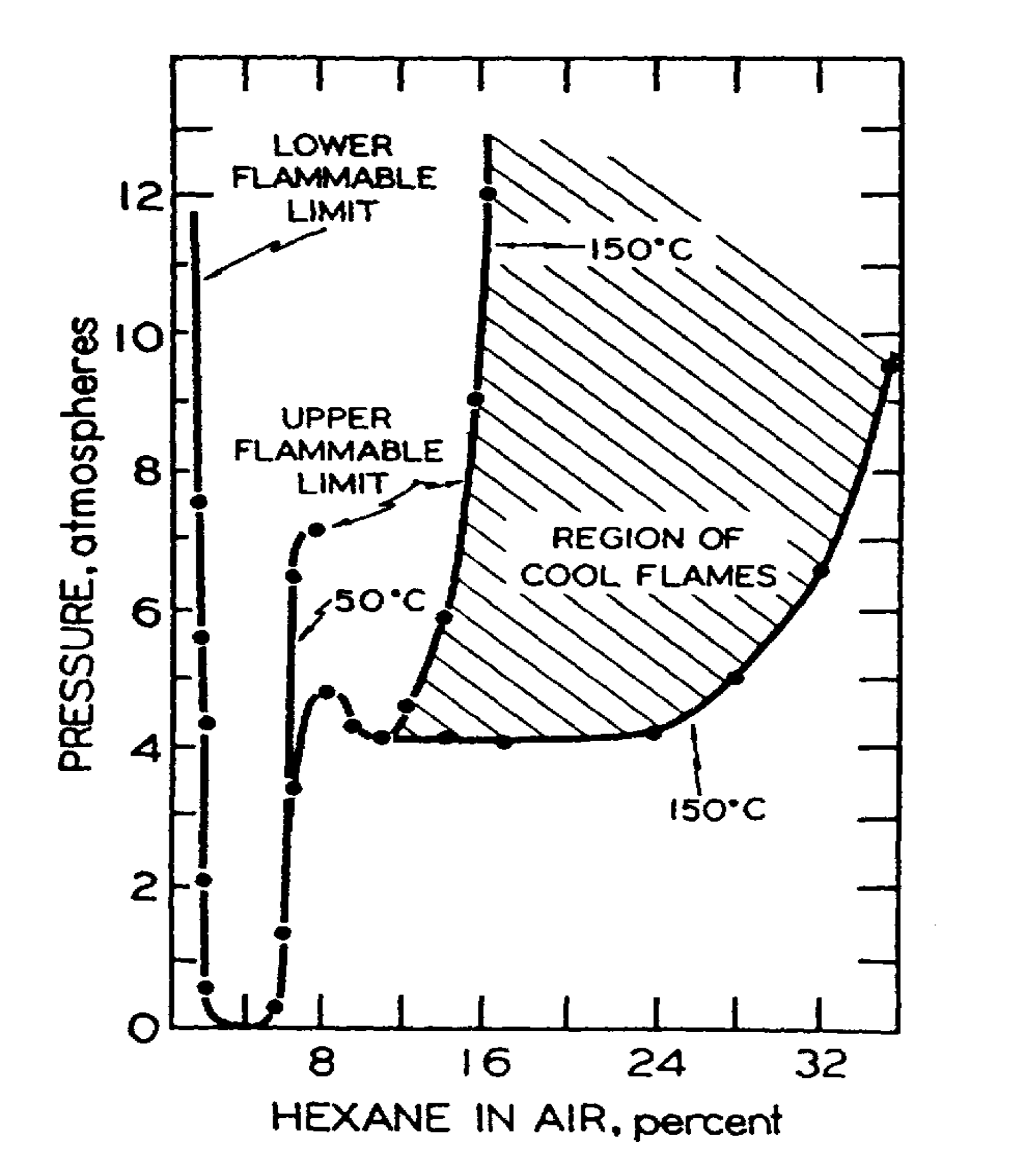
Effect of pressure, temperature, and fuel concentration on Flammability Limits



Flammability limits (FL) are affected by

1) Temperature
2) Pressure
3) Fuel type and concentration
4) Oxidiser type and concentration
5) Size of vessel and dimension
6) Ignition type and strength
7) Direction of flame propagation
8) Turbulence
9) Impurities
10) Catalytic material
11) Ignition criterion
12) Cool flame phenomena (at elevated conditions)

Importance of reaction kinetic knowledge



GENERAL COMBUSTON KINETICS

For any hydrocarbon at stiochiometric concentration

$$C_xH_yO_z + (x+y/4-z/2)O_2 \rightarrow xCO_2 + y/2H_2O$$

The general oxidation scheme shows only the **overall reaction** and contains **absolutely no information** about the intermediate species and the oxidation mechanism

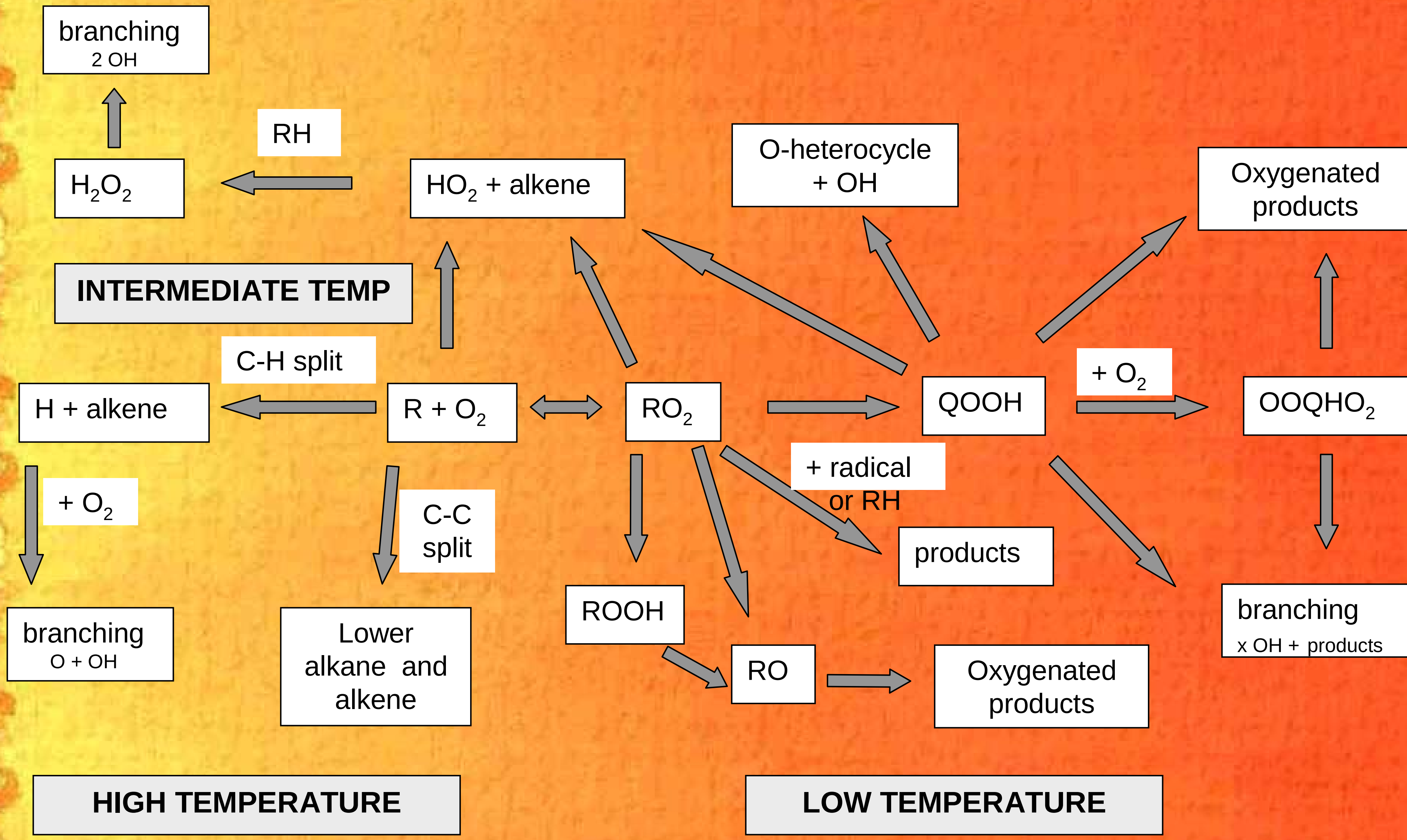
Therefore

1) The oxidation path and intermediate products are unknown
2) Reaction time is unknown

The oxidation reactions can be divided into three mechanisms namely: *initiation, propagation* and *termination*

We have experts in the audience on this subject

General oxidation scheme with respect to temperature



WHAT CAN BE DONE?

WHAT IS THE PROPER WAY FORWARD?

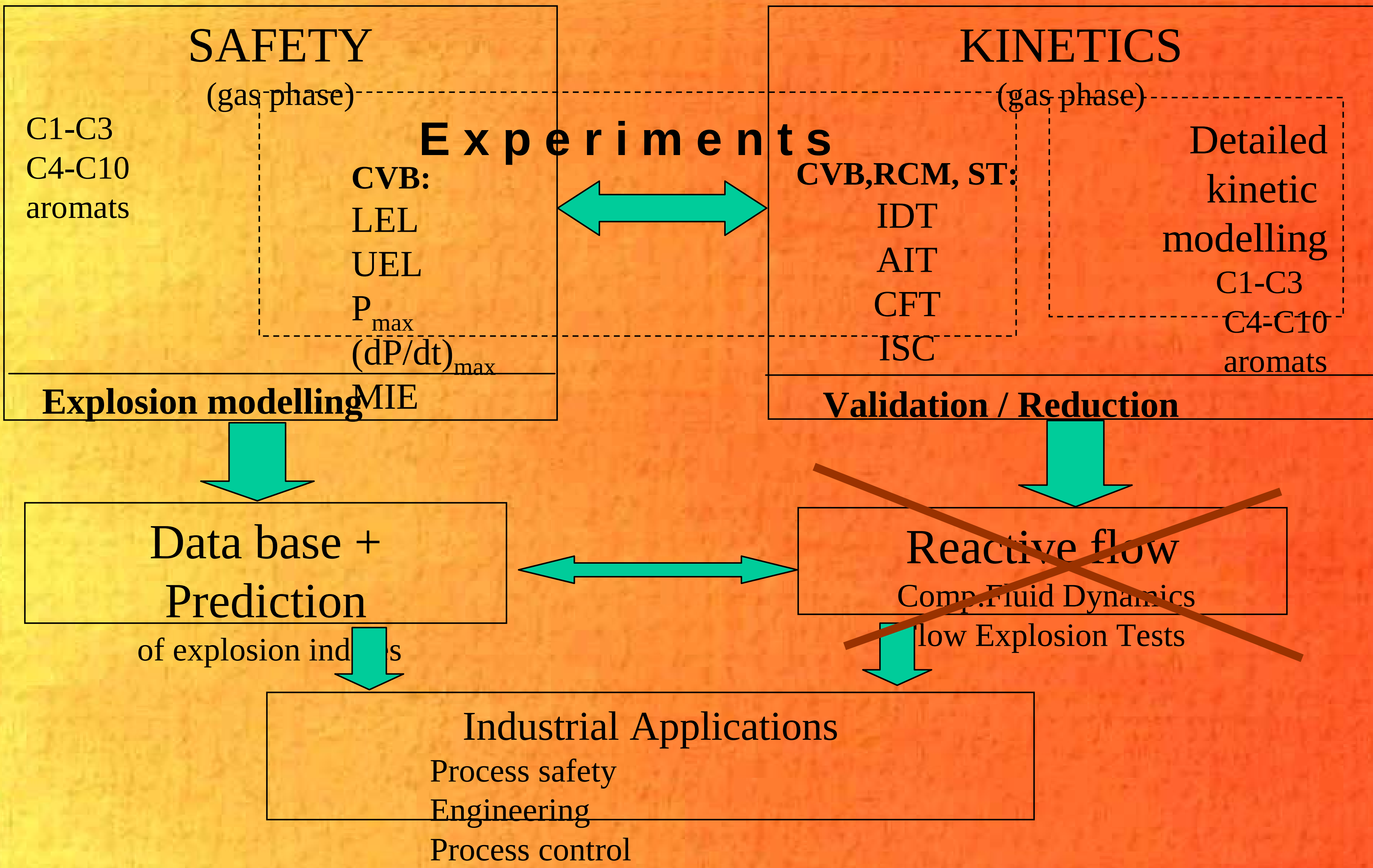
BAM, INERIS, WUT, UK, BASF, TUW, TUD

CNRS, VUB, UL, TUD

Constrain: Gas phase kinetics (no heterogeneous reactions)

next

SAFEKINEX work overview



CVB = Constant Volume Bomb; RCM = Rapid Compression Machine
LEL = Lower Explosion Limit ; UEL Upper Explosion Limit
IDT = Induction Time; AIT = Auto-Ignition Temperature;
CFT = Cool Flame Temperature; ISC = Identified Species Concentration