EXPERIMENTAL AND NUMERICAL STUDY OF THE CHEMICAL REACTIONS INVOLVED IN THE IN SITU COMBUSTION (ISC) PROCESS

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INTERNAL COMBUSTION ENGINE (ICE)



From the model T by Ford in the early 1900s the internal combustion engine, associated with the automobile, was considered an excellent idea. Fuels were burned to move a piston and power an automobile

In the 60s automobiles were considered as a source of pollutants such as NOx, SOx, CO, HCs and CO₂ They were also labelled as high-fuel consumers with low efficiency



 $2C_8H_{18} + 25O_2 \rightarrow 16CO_2 + 18H_2O$

 $iC_8H_{18} \to tC_4H_9 + tC_4H_9$ $iC_8H_{18} \to yC_7H_{15} + CH_3$ $iC_8H_{18} + H \rightarrow cC_8H_{17} + H_2$ $iC_8H_{18} + \dot{H} \rightarrow b\dot{C}_8H_{17} + H_2$ $iC_8H_{18} + H \rightarrow dC_8H_{17} + H_2$ $iC_8H_{18} + OH \rightarrow aC_8H_{17} + H_2$ $i \stackrel{\bullet}{C}_3 H_7 \rightarrow C_3 H_6 + H$ $d\overset{\bullet}{C}_8 H_{17} \rightarrow C_3 H_6 + neo\overset{\bullet}{C}_5 H$

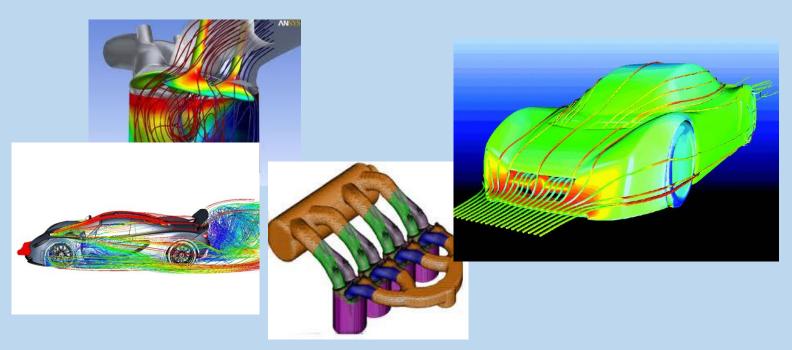
 $p \, \dot{C}_7 \, H_{15} \rightarrow C_3 H_6 + t \, \dot{C}_4 \, H_9$

 $iC_4H_9 \rightarrow C_3H_6 + CH_3$ $iC_8H_{18} + OH \rightarrow aC_8H_{17} + H_2O$ $a\overset{\bullet}{C}_8 H_{17} \rightarrow iC_4 H_8 + i\overset{\bullet}{C}_4 H_9$ $c\overset{\bullet}{C}_8H_{17} \rightarrow iC_4H_8 + t\overset{\bullet}{C}_4H_9$ $tC_4H_9 \rightarrow iC_4H_8 + H$ $a\overset{\bullet}{C}_8 H_{17} \rightarrow iC_4 H_8 + i\overset{\bullet}{C}_4 H_9$

 $iC_8H_{18} + \dot{H} \rightarrow a\dot{C}_8H_{17} + H_2 d\dot{C}_8H_{17} \rightarrow C_3H_6 + neo\dot{C}_5H_{11} iC_8H_{18} \rightarrow neo\dot{C}_5H_{11} + i\dot{C}_3H_7$ $\stackrel{\cdot}{C}H_3 + \stackrel{\cdot}{C}H_3 \rightarrow C_2H_6$ $iC_4H_7 + \dot{C}H_3 \rightarrow aC_5H_{10}$ $i, t \stackrel{\bullet}{C_4} H_9 + O_2 \rightarrow i C_4 H_8 + H \stackrel{\bullet}{O_2} \quad i C_4 H_7 \rightarrow C_3 H_4 - a + \stackrel{\bullet}{C} H_3$ $c \overset{\bullet}{C}_{8} H_{17} \rightarrow i C_{4} H_{8} + t \overset{\bullet}{C}_{4} H_{9}$ neo $\overset{\bullet}{C}_{5} H_{11} \rightarrow i C_{4} H_{8} + i \overset{\bullet}{C} H_{3}$

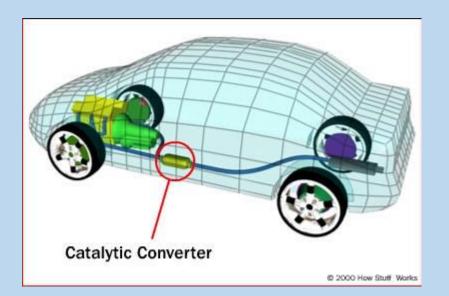
Species:860 Reactions:3600

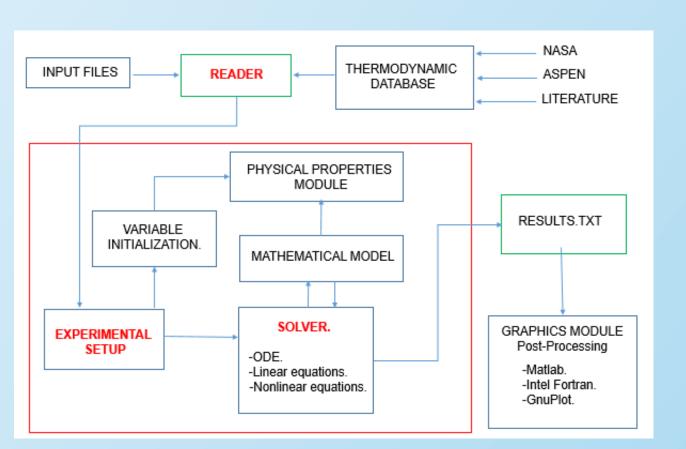
Improvement of automobile was obtained in part thanks to a thorough understanding of the chemistry associated to the process. Current reaction mechanisms exceed 1000 $_{7}H_{15} \rightarrow iC_{4}H_{8} + i\overset{\bullet}{C}_{3}H_{7}$ $\dot{C}_4 H_9 \rightarrow i C_3 H_6 + \dot{C} H_3$ reactions and 500 species



Advanced modelling by computational fluid dynamics (CFD) has been fundamental as well in improving fuel efficiency and reducing emissions in a car

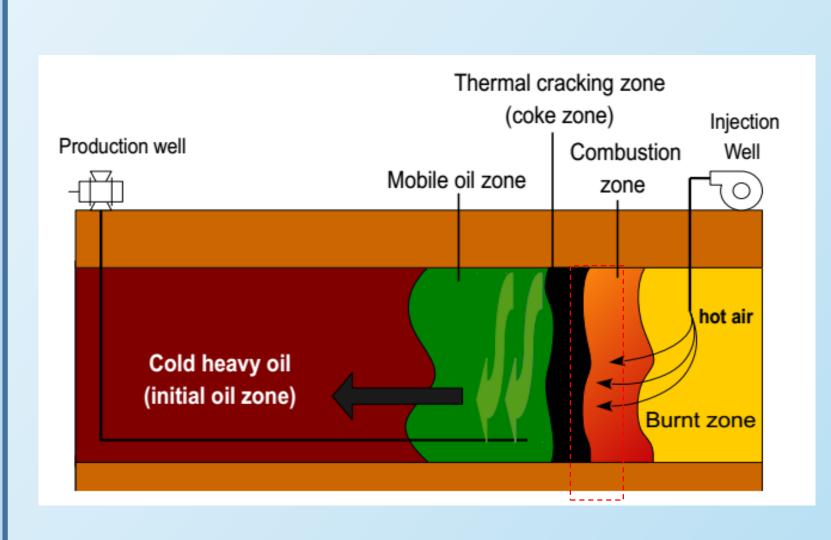
Research eventually led to devices such as the three-way catalytic converter that significantly reduced emissions and allowed the extended use of automobiles





The CFD and experimental efforts are supported by the development of a simulation toolbox with the ability to obtain a solution for different experimental setups, operating condition or different physical models with emphasis in the chemistry and thermochemical properties of the involved species

IN SITU COMBUSTION (ISC)



In situ combustion has been regarded as a clever idea to recover heavy crude by generating a combustion front, increasing temperature and decreasing viscosity

The future of ISC combustion as a technique for enhanced oil recovery is currently being decide by research, both fundamental and applied

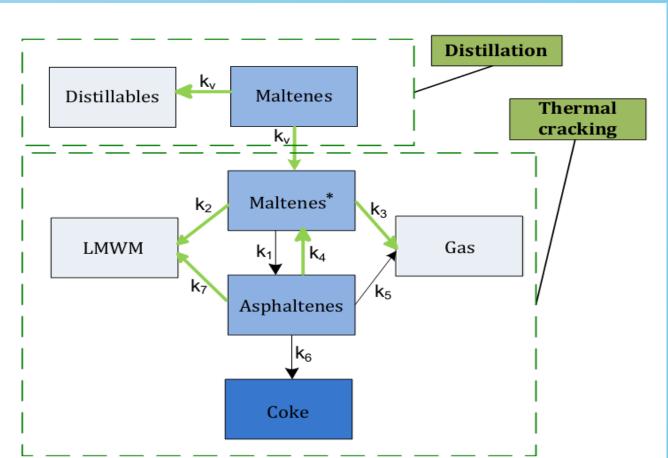


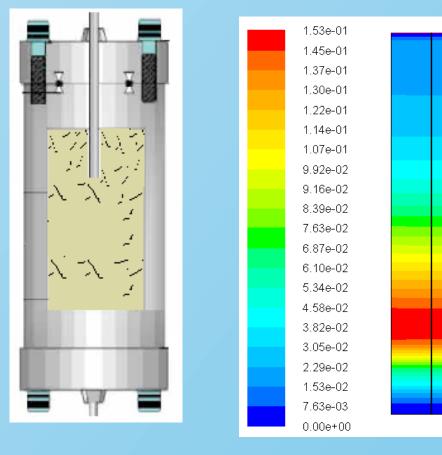
LTO: $Maltenes + 3.431O_2 \longrightarrow 0.4726 Asphaltenes$ $Asphaltenes + 7.513O_2 \longrightarrow 101.539Coke$ $Maltenes \longrightarrow 0.372 Asphaltenes$ Pyrolisys: $Asphaltenes \longrightarrow 83.223Coke$ $Asphaltenes \longrightarrow 37.683Gas$ $Coke + 1.232O_2 \longrightarrow CO_x + 0.565H_2O$ HTO:

Current reaction mechanisms that describe ISC are too general

WE AIM AT UNDERSTANDING AND IMPROVING ISC AS THE AUTOMOBILE INDUSTRY IMPROVED THE ICE

Experiments in a horizontal tube indicated that during the thermal cracking of crude oil distillation and the conversion of the different fractions to intermediate compounds are important





CFD simulations showed differences in O₂ concentration along a kinetic cell. This suggests that the use of a perfectly-stirred reactor model to process the experimental data obtained in a kinetic cell can cause significant errors

The authors would like to acknowledge the financial support from the Colombian Science Foundation (COLCIENCIAS), and the Colombian state oil company (ECOPETROL S.A.) under contract No. 0264-2013.