CM1404

SMARTCATs

UNIVERSITÉ LIBRE DE BRUXELLES
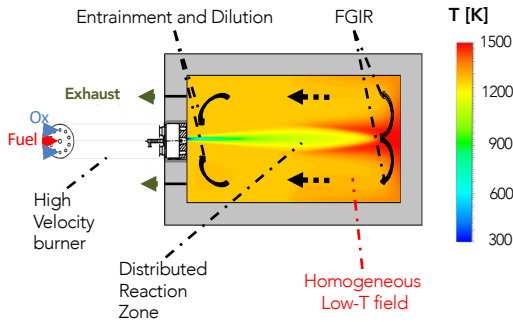
POLITECNICO MILANO 1863

urn combustion 2.0

Hierarchical development of OPTImised kinetic Mechanisms for Advanced combustion technoLogies (HOPTIMAL)
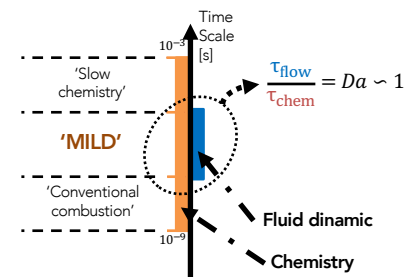
A. Bertolino[1], A.Frassoldati[2], A.Parente[1]

[1]Aero Thermo Mechanics Department, Université Libre De Bruxelles;
[2]CRECK modelling, Chemical Engineering Departement ,Politecnico di Milano;

Turbulence/chemistry interaction in MILD combustion

Entrainment and Dilution
FGIR
Exhaust
Ox
Fuel
High Velocity burner
Distributed Reaction Zone
Homogeneous Low-T field
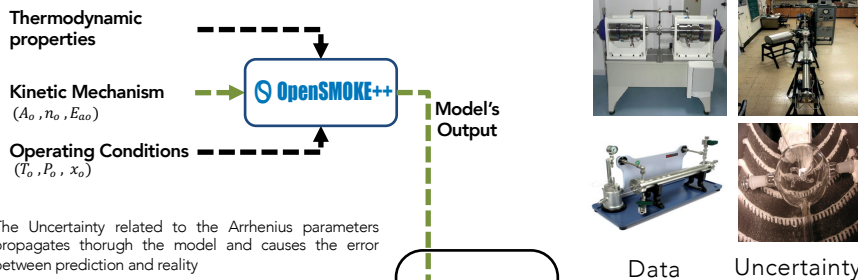
T [K]
1500
1200
900
600
300

In MILD regime the entrainment of combustion products due to flue gas internal recirculation causes the chemistry to be delayed with respect to conventional combustion. For this reason, the time scales of fluid dinamic and chemistry overlap, that's why higher complexity is associated with modelling the process. **Detailed kinetics is needed** for chemistry to be correctly coupled with turbulence, but existing mechanisms are not suited to reproduce higly diluted reactive flows. Without getting rid of the latters, **it is possible to optimise them applying Uncertainty quantification methods to classical kinetic studies on canonical reactors.**

Time Scale [s]
10^{-3}
'Slow chemistry'
'MILD'
'Conventional combustion'
10^{-9}

$\frac{\tau_{flow}}{\tau_{chem}} = Da \sim 1$

Fluid dinamic
Chemistry

Methodology

Numerical simulation of canonical reactors' behaviour in MILD-like conditions will drive the validation process of the emerging clean fuels' reaction mechanisms. To achieve this objective the comparison with experimental data from literature on Rapid Compression Machines, Shock Tubes, Plug Flow Reactors and Well Stirred Reactors is needed to drive the process.
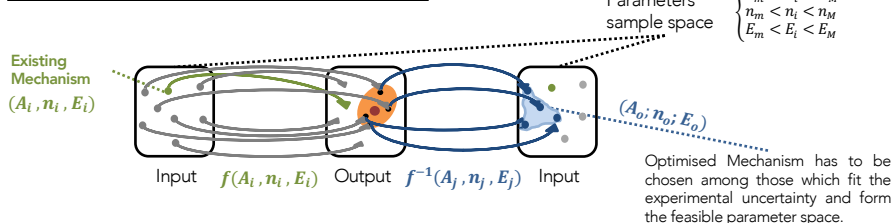
Thermodynamic properties

Kinetic Mechanism
(A_o , n_o , E_{ao})

OpenSMOKE++

Model's Output

Operating Conditions
(T_o , P_o , x_o)

The Uncertainty related to the Arrhenius parameters thorugh the model and causes the error between prediction and reality
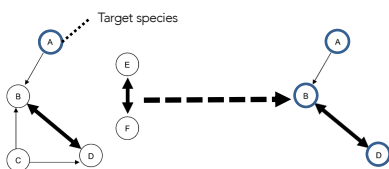
$R_i \pm \varepsilon_R$

Δ

Data   Uncertainty

Physical output space

$R_i = A T^n e^{\left[-\frac{E}{RT}\right]} \prod_i^N C_i$

UQ INVERSE PROBLEM FOR OPTIMISATION

Parameters sample space
$\begin{cases} A_m < A_i < A_M \\ n_m < n_i < n_M \\ E_m < E_i < E_M \end{cases}$

Existing Mechanism
(A_i , n_i , E_i)

$(A_o; n_o; E_o)$

Input $f(A_i , n_i , E_i)$ Output $f^{-1}(A_j , n_j , E_j)$ Input

Optimised Mechanism has to be chosen among those which fit the experimental uncertainty and form the feasible parameter space.

DRG-like METHOD FOR MECHANISMS REDUCTION

Target species

A
E
B
F
C
D

A
B
D

$I_{AJ} = \frac{\sum_{i=1}^{n} |\upsilon_{A,i} \cdot r_i \cdot \delta_{Ji}|}{\sum_{i=1}^{n} |\upsilon_{A,i} \cdot r_i|} > \varepsilon$ (threshold value)

$\delta_{Ji} = \begin{cases} 1 & \text{If the J-th species participate to i-th reaction with A} \\ 0 & \text{Otherwise} \end{cases}$

Only strongly linked species will be kept into the final mechanisms

Hierarchical Development

N_2
CO_2
H_2O

CH_4
CH_3OH
H_2/CO
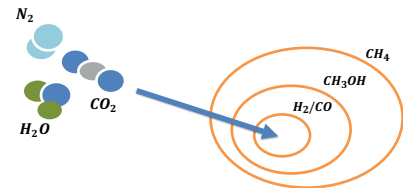
Syngas, Biogas, Natural gas and other Smart energy carriers are the subject of this work. They are mixtures of simpler pure fuels. In order to be predictive for a composed combustible, a kinetic mechanism should be first validated for the pure compounds, which compose it. Also the high dilution level effect should be optimised and validated hierachically.

Objectives and Plan

1. Collect data and related Uncertainties from Literature on Canonical reactors;
2. Reproduce the aforementioned data sets with OpenSMOKE++, and perform sensitivity analysis to individuate important reactions to for the specific conditions;
3. Use the sensitivity coefficient to perform optimisation through Uncertainty quantification based methods in Dakota;
4. Reduce optimised mechanisms to decrease computational efforts for future CFD studies with DRG-like methods in DoctorSMOKE++;
5. Validate a model on Pilot-scale data coupling kinetic and turbulence model in OpenFOAM.

Acknowledgements

References

[1] J.A. Wunning and J.G. Wunning, Prog. Energy Comb. Sci. , (1997)
[2] A. Cavaliere and M. de Joannon, Prog. Energy Comb. Sci. , (2004)
[3] B.B. Dally et al. , Combustion and Flame, (2004)
[4] R. Fox, Cambridge Uni press, (2002)
[5] A. Cuoci et al. , Computer Physics Communications , (2015)
[6] T. Nagy , T. Turányi, Wiley online library, (2010)
[7] T. Nagy et al. , Combustion and Flame, (2015)
[8] M. Fürst et al. , INTO THE PROCESS OF PUBLICATION, (2017)
[9] T. Lu , C.K. Law, Proc. of the Combu. Inst. , (2005)
[10] E. Ranzi , Prog . Energy Comb. Sci. , (2012)