Tabulation of Dynamic Adaptive Chemistry: A global approach to include detailed mechanisms in engine simulations

Francesco Contino, Hervé Jeanmart
Université catholique de Louvain, Belgium

Tommaso Lucchini, Gianluca D'Errico
Politecnico di Milano

11th July 2011
Tabulation of Dynamic Adaptive Chemistry: A global approach to include detailed mechanisms in engine simulations

Including kinetic mechanisms

TDAC : how it works

Perspectives
Tabulation of Dynamic Adaptive Chemistry: A global approach to include detailed mechanisms in engine simulations

Including kinetic mechanisms

TDAC: how it works

Perspectives
The integration of a large system of non-linear stiff ODE is time-consuming

\[
\psi(t) = (Y_i, T, p) \quad \text{CFD} \quad \tilde{S}(\psi(t)) \quad \text{Chemical} \quad Y_i(t) = S(\psi(t))
\]

\[
\dot{Y}_i(t) = \tilde{S}(\psi(t)) + M(\psi(t))
\]

\[
\dot{Y}_i(t) = S(\psi(t))
\]

For comprehensiveness, more species is better

For computational cost, less species is better
When the number of species increases, the network becomes more complex

\[
\begin{align*}
C_7H_{16} + 11O_2 & \Rightarrow 7CO_2 + 8H_2O \\
CO + O + M &= CO_2 + M \\
CO + OH &= CO_2 + H \\
CO + O_2 &= CO_2 + O \\
HO_2 + CO &= CO_2 + OH \\
H_2 + O_2 &= OH + OH \\
H_2 + OH &= H_2O + H \\
O + OH &= O_2 + H \\
O + H_2 &= OH + H \\
H + HO_2 &= O + H_2O \\
O + OH + M &= HO_2 + M \\
H + O_2 + M &= HO_2 + M \\
H + O_2 + O_2 &= HO_2 + O_2 \\
H + O_2 + H_2O &= HO_2 + H_2O \\
H + O_2 + N_2 &= HO_2 + N_2 \\
OH + HO_2 &= H_2O + O_2 \\
H + HO_2 &= OH + OH \\
O + HO_2 &= O_2 + OH \\
OH + OH &= O + H_2O \\
H + H + M &= H_2 + M \\
H + H + H_2 &= H_2 + H_2 \\
H + H + H_2O &= H_2 + H_2O \\
H + H + CO_2 &= H_2 + CO_2 \\
H + OH + M &= H_2O + M \\
H + O + M &= OH + M \\
O + O + M &= O_2 + M \\
H + HO_2 &= H_2 + O_2 \\
HO_2 + HO_2 &= H_2O_2 + O_2 \\
OH + OH + M &= H_2O_2 + M \\
H_2O_2 + H &= HO_2 + H_2 \\
H_2O_2 + OH &= H_2O + HO_2 \\
H_2O_2 + H &= H_2O + OH \\
H_2O_2 + O &= H_2O + O_2 \\
H_2O_2 + O &= OH + HO_2 \\
H_2 + HO_2 &= H_2O + OH
\end{align*}
\]

11 species, 45 reactions
When the number of species increases, the network becomes more complex.
When the number of species increases, the network becomes more complex.
Tabulation of Dynamic Adaptive Chemistry: A global approach to include detailed mechanisms in engine simulations

Including kinetic mechanisms

TDAC: how it works

Perspectives
TDAC is a new layer between the CFD and the ODE solvers
TDAC is a new layer between the CFD and the ODE solvers
TDAC is the coupling of two simplification methods

- **In Situ Adaptive Tabulation**
  - Solution storage/retrieval algorithm
  - (Pope, 1997)

- **Dynamic Adaptive Chemistry**
  - Mechanism reduction method
  - (Liang, 2009)
TDAC is the coupling of two simplification methods

ISAT tries to retrieve previously stored results
DAC reduces the mechanism at runtime

TDAC achieves a significant speed-up factor

- TDAC: 374 cells, 561 species, speed-up = 150
- DAC: 30
- ISAT: 25
TDAC and direct integration are in good agreement
TDAC and experimental data are in good agreement.

Symbol: computed
Line: measured

exp.: Hessel et al., 2008

Speed-up factor 500
TDAC takes advantage of the synergy between DAC and ISAT
Tabulation of Dynamic Adaptive Chemistry: A global approach to include detailed mechanisms in engine simulations

Including kinetic mechanisms

TDAC: how it works

Perspectives
The next step is to use it in many different applications

Apply TDAC to simulations of
conventional engines
full engine cycles
Mass fraction

CAD ATDC

CO₂

fuel (NC₇H₁₆)

CO₂
Perspectives for TDAC

Apply TDAC to advanced simulations
conventional engines
full engine cycles

Further analyze the component of TDAC
optimize the interactions
add new layers
Different reduction methods in TDAC are compared with direct integration in a simple case

HCCI combustion

Axisymmetric mesh: 1350 cells

Iso-octane mech.: 874 species

Diagram:

- CFD
- ISAT
- Chemical
Overall, DRG and DAC perform better.
Perspectives for TDAC

Apply TDAC to advanced simulations
conventional engines
full engine cycles

Further analyze the component of TDAC
optimize the interactions
add new layers

Use graph and network theory
IC8H18

Fuel

O2

Major

Minor

Disabled

A + B ↔ C

A

B

C
Tabulation of Dynamic Adaptive Chemistry: A global approach to include detailed mechanisms in engine simulations

Including kinetic mechanisms

TDAC: how it works

Perspectives
Try it... and use it for free

http://twitter.com/TDAC_News

francesco.contino@uclouvain.be

git://github.com/fcontino/TDAC.git