Americo Barbosa da Cunha Junior

Reduction of Complexity in Combustion Thermochemistry

DISSERTAÇÃO DE MESTRADO

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Dissertação de Mestrado

Dissertation presented to the Postgraduate Program in Mechanical Engineering of the Departamento de Engenharia Mecânica do Centro Técnico Científico da PUC–Rio, as partial fulfillment of the requirements for the degree of Mestre em Engenharia Mecânica.

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Abstract

Cunha, Americo Barbosa; Figueira da Silva, Luís Fernando. **Reduction of Complexity in Combustion Thermochemistry**. Rio de Janeiro, 2010. 134p. Dissertação de Mestrado — Departamento de Engenharia Mecânica, Pontifícia Universidade Católica do Rio de Janeiro.

The development of computational models for the numerical simulation of chemically reacting flows operating in the turbulent regime requires the solution of partial differential equations that represent the balance of mass, linear momentum, chemical species and energy. Moreover, the chemical reactions of the model may require a detailed reaction mechanism for the description of the physicochemical phenomena involved. One of the biggest challenges is the stiffness of the numerical simulation of these models and the nonlinear nature of species rate of reaction. This dissertation presents an overview of the main techniques available in the literature for the development of reduced models of chemical kinetics, particularly for the combustion, as well as the techniques for efficient computation of the chemically reacting flows models. After a presentation of the associated mathematical formulation, the methodology dubbed *in situ* adaptive tabulation (ISAT) is implemented and its accuracy, efficiency and memory usage are evaluated in the simulation of homogeneous stirred reactor models. The combustion of carbon monoxide with oxygen and methane with air mixtures is considered, which detailed reaction mechanisms involve 4 and 53 species, 3 and 325 reactions respectively. The results of these simulations indicate that the development implementation of the ISAT technique has a absolute global error of less than 1%. Moreover, the ISAT technique provided gains, in terms of computational time, of up to 80% when compared to the direct integration of the full chemical kinetics. However, in terms of memory usage the present implementation of ISAT technique was found to be excessively demanding.

Keywords

combustion modelling. detailed thermochemistry. reduced model. adaptive tabulation.

Resumo

Cunha, Americo Barbosa; Figueira da Silva, Luís Fernando. **Redução de Complexidade da Cinética Química da Combustão**. Rio de Janeiro, 2010. 134p. Dissertação de Mestrado — Departamento de Engenharia Mecânica, Pontifícia Universidade Católica do Rio de Janeiro.

O desenvolvimento de modelos computacionais para simulação de escoamentos reativos operando em regime de turbulência requer a solução das equações diferenciais parciais que representam os balanços de massa, quantidade de movimento linear, espécies químicas e energia. Além disso, as reações químicas do modelo necessitam de um mecanismo cinético detalhado para descrição dos fenômenos físico-químicos associados. Um dos maiores desafios encontrados é a rigidez da simulação numérica desses modelos e a natureza não linear do termo de produção das espécies químicas. Esta dissertação apresenta uma revisão das principais técnicas disponíveis na literatura para o desenvolvimento de modelos reduzidos de cinética química, em particular para a combustão, bem como de técnicas para solução eficiente dos modelos de escoamentos reativos. Após uma apresentação da formulação matemática associada, a metodologia denominada tabulação adaptativa *in situ* (ISAT) é implementada e avaliada quanto a sua acurácia, eficiência e uso de memória na simulação de alguns modelos de reator homogêneo agitado. Avalia-se a combustão de misturas de monóxido de carbono/oxigênio e metano/ar cujos mecanismos cinéticos tem 4 e 53 espécies, 3 and 325 reações respectivamente. Os resultados destas simulações indicam que a presente implementação da técnica ISAT tem erro relativo global inferior a 1%. Além disso, a técnica ISAT propiciou ganhos, em termos de tempo computacional, de até 80% quando comparado a simulação direta da cinética detalhada. Entretanto, em termos de utilização da memória, a implementação desenvolvida da técnica ISAT se mostrou excessivamente exigente.

Palavras–chave

modelagem da combustão. cinética química detalhada. modelo reduzido. tabulação adaptativa.

Contents

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Nomenclature

Upper-case Roman

$\boldsymbol{A}(\boldsymbol{\phi}, t)$	mapping gradient matrix
$\boldsymbol{B}$	scaling matrix
$\boldsymbol{G}$	rank-one modification matrix
$\boldsymbol{I}$	identity matrix
$\boldsymbol{J}$	Jacobian matrix of $\boldsymbol{N}$
$\boldsymbol{L'}$	new EOA Cholesky matrix
$\boldsymbol{L}$	EOA Cholesky matrix
$\boldsymbol{N}$	nonlinear system of algebraic equations
$\boldsymbol{R}(\boldsymbol{\phi}, t)$	reaction mapping of $\boldsymbol{\phi}$
$\boldsymbol{R}^c(\boldsymbol{\phi}, t)$	constant approximation for $\boldsymbol{R}(\boldsymbol{\phi}, t)$
$\boldsymbol{R}^l(\boldsymbol{\phi}, t)$	linear approximation for $\boldsymbol{R}(\boldsymbol{\phi}, t)$
$\boldsymbol{S}(\boldsymbol{\phi}, t)$	reaction vector
$\boldsymbol{U}$	real square orthogonal matrix
$\boldsymbol{V}$	real square orthogonal matrix
$\mathcal{A}$	accessed region
$\mathcal{C}$	composition space
$\mathcal{M}_i$	i-th chemical species symbol
$\mathcal{R}$	realizable region
$\overline{W}$	mean molar mass
$\widetilde{\boldsymbol{A}}$	modification of $\boldsymbol{A}$
$A_{ij}(\boldsymbol{\phi}, t)$	components of $\boldsymbol{A}(\boldsymbol{\phi}, t)$
A_j	j-th reaction pre-exponential factor
C	mixture concentration
C_i	i-th chemical species molar concentration
E_j	j-th reaction activation energy
H_i^o	i-th chemical species enthalpy of formation
K	number of time steps

K_{c_j} j-th reaction equilibrium in concentration units

K_{p_j} j-th reaction equilibrium in pressure units

N_A Avogadro number

R universal gas constant

$R_i(\boldsymbol{\phi}, t)$ i-th component of $\boldsymbol{R}(\boldsymbol{\phi}, t)$

S_i^o i-th chemical species entropy in standard state

T temperature

T^o temperature at standard state

V system volume

W_i i-th chemical species molar mass

X_i i-th chemical species molar fraction

X_{Fu} fuel molar fraction

X_{Ox} oxidizer molar fraction

Y_i i-th chemical species mass fraction

Lower-case Roman

$\boldsymbol{v}$ cutting plane normal vector

$\dot{m}$ mass flow rate

$\mathbf{u}$ velocity field

$\widetilde{l}_i$ modified length of EOA in i-th direction

a cutting plane scalar

c_{p_i} i-th chemical species specific heat

h specific enthalpy

h_i i-th chemical species specific enthalpy

h_i^o i-th chemical species specific enthalpy of formation

k_j j-th reaction rate constant

l_i half-length of EOA in i-th principal direction

m system total mass

m_i i-th chemical species mass

n system total number of moles

n_i i-th chemical species number of moles

n_r number of elementary reactions

n_s number of chemical species

n_ϕ number of composition components

n_A number of additions

n_{DE} number of direct evaluations

n_{DI} number of direct integrations

n_G number of growths

n_{in} number of particles to input the system

n_L number of leaves

n_N number of nodes

n_{pair} number of particles for pairing

n_p number of reactor particles

n_R number of retrieves

n_{tab} number of entries in the binary search tree

p pressure

p^o pressure at the standard state

q order of BDF method

r_j j-th reaction rate

t time

t_0 initial time

t_n n-th time instant

u_r machine unit roundoff

w_i i-th error weight

Upper-case Greek

$\mathbf{\Gamma}(t)$ mixing vector

$\mathbf{\Sigma}$ real square diagonal matrix

$\Delta\tau$ time interval

ΔH_j^o j-th reaction net change in enthalpy

ΔS_j^o	j-th reaction net change in entropy
Δt	time step
Δt_n	n-th time step
Γ_ρ	continuity equation right hand side term
$\Gamma_{\mathbf{u}}$	momentum equation right hand side term
Γ_h	energy equation right hand side term
Γ_{Y_i}	i-th chemical species equation right hand side term
Ω_i	i-th chemical species equation chemical source term
Φ	equivalence ratio
$\widetilde{\mathbf{\Sigma}}$	modification of $\mathbf{\Sigma}$

Lower-case Greek

α_j	coefficients of BDF method
β_j	j-th reaction temperature exponent
$\boldsymbol{\epsilon}$	vector with the local truncation errors
$\widetilde{\boldsymbol{\phi}}$	transformed $\boldsymbol{\phi}$
$\boldsymbol{\phi}$	composition
$\boldsymbol{\phi}_0$	initial composition
$\boldsymbol{\phi}_q$	query composition
$\boldsymbol{\phi}_{mix}$	solution of the mixing system
$\boldsymbol{\zeta}$	constant vector
$\boldsymbol{\zeta}_1$	constant vector
$\boldsymbol{\zeta}_2$	constant vector
$\delta\boldsymbol{\phi}$	composition displacement
$\dot{\omega}_i$	i-th chemical species reaction rate
ϵ_i	i-th component of $\boldsymbol{\epsilon}$
ϵ_G	global error of ISAT
γ	rank-one modification constant
κ	lower bound
$\nu_{ij}^{''}$	reverse stoichiometric coefficients

ν'_{ij} forward stoichiometric coefficients

ν_{ij} overall stoichiometric coefficients

$\phi_i(t_n)$ i-th component of $\boldsymbol{\phi}(t_n)$

$\widetilde{\phi}_q$ Euclidean norm of $\widetilde{\boldsymbol{\phi}}_q$

ψ generic property

ρ mixture density

ρ_i i-th chemical species partial density

σ_i singular values of $\boldsymbol{A}$

τ_m mixing time scale

τ_p pairwise time scale

τ_r residence time

τ_A average time spent at each addition

τ_{DE} average time spent at each direct evaluation

τ_{DI} average time spent at each direct integration

τ_G average time spent at each growth

τ_R average time spent at each retrieve

ε local error of linear approximation

ε_{ψ_r} relative local error of ψ

ε_{abs} solver absolute tolerance

ε_g absolute global error of ISAT

ε_{rel} solver relative tolerance

ε_{tol} error tolerance of ISAT

$\widetilde{\sigma}_i$ singular values of $\widetilde{\boldsymbol{A}}$

Superscripts

* dimensionless quantity

$^\mathtt{T}$ transposition operation

$^{(j)}$ index of the j-th particle

$^+$ forward reaction

$^-$ reverse reaction

^{m}	m-th approximation

Subscripts

$_{0}$	initial condition
$_{DI}$	direct integration calculation
$_{eq}$	equilibrium condition
$_{in}$	input condition
$_{ISAT}$	ISAT calculation
$_{st}$	stoichiometric condition

Other Symbols

$ceil\,(\cdot)$	ceil function
$\int$	integral
$\frac{\partial}{\partial t}$	partial derivative with respect to t
$\prod$	product
$\sum$	summation
$\frac{d}{dt}$	total derivative with respect to t
$\equiv$	definition
$\langle\cdot\rangle_{\infty}$	function maximum
$\langle\cdot\rangle_{M}$	function mean
$\langle\cdot\rangle$	ensemble average
$\|\|\cdot\|\|_{wrms}$	weighted root mean square norm
$\|\|\cdot\|\|_{2}$	Euclidean norm
$\#\,(\texttt{data})$	memory cost of `data`
$\mathcal{O}(\cdot)$	big O notation
$\langle\cdot'^{2}\rangle$	ensemble variance

Abbreviations

ANN	artificial neural network
CSP	computational singular perturbation

D/R	dimension reduction
DI	direct integration
DRG	directed relation graph
EOA	ellipsoid of accuracy
ICE-PIC	invariant constrained equilibrium edge pre-image curve
IEM	interaction by exchange with the mean
ILDM	intrinsic low-dimensional manifold
ISAT	*in situ* adaptive tabulation
LES	large eddy simulation
LUT	look-up table
ODE	ordinary differential equation
PaSR	partially stirred reactor
PDF	probability density function
PMSR	pairwise mixing stirred reactor
POD	proper orthogonal decomposition
PRISM	piece-wise reusable implementation of solution mapping
PSR	perfect stirred reactor
QSSA	quasi-steady state approximation
RANS	Reynolds averaged Navier-Stokes
RCCE	rate-controlled constrained equilibrium
RM	repro-modelling
S/M	skeletal mechanism
S/R	storage/retrieval
SA	sensitive analysis
SVD	singular value decomposition

Chemical Species

C_2H_2	acetylene
C_2H_4	ethylene
CH_2O	formaldehyde

CH_3	methyl radical
CH_3O	methoxy radical
CH_4	methane
CO	carbon monoxide
CO_2	carbon dyoxide
H	hydrogen atom
H_2	hydrogen
H_2O	water
H_2O_2	hydrogen peroxide
HCO	formyl radical
HO_2	hydroperoxy radical
M	third body
N_2	nitrogen
NO_x	nitrogen oxide
O	oxygen atom
O_2	oxygen
OH	hydroxyl radical

"In questions of science, the authority of a thousand is not worth the humble reasoning of a single individual."

Galileo Galilei (1564 – 1642) , *Third letter on sunspots to Mark Wesler* .