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**Reduction of Complexity in
Combustion Thermochemistry**

DISSERTAÇÃO DE MESTRADO

DEPARTAMENTO DE ENGENHARIA MECÂNICA

Postgraduate Program in Mechanical Engineering



Americo Barbosa da Cunha Junior

**Reduction of Complexity in Combustion
Thermochemistry**

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.

Advisor: Prof. Luís Fernando Figueira da Silva

Rio de Janeiro
August 2010



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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

1	Introduction	23
1.1	Historical and Economical Aspects	23
1.2	Combustion Applied to Industrial Devices	24
	<i>Industrial Process Furnaces</i>	24
	<i>Gas Turbines</i>	25
1.3	Fundamental Challenges	26
1.4	Objectives of this Dissertation	27
1.5	Outline of this Dissertation	27
2	Literature Review	28
2.1	Introduction to the Reduction Approaches	28
2.2	Reduction to Skeleton Mechanisms	28
	<i>Sensitivity Analysis</i>	29
	<i>Proper Orthogonal Decomposition</i>	30
	<i>Directed Relation Graph</i>	31
2.3	Dimension Reduction	32
	<i>Reaction Lumping</i>	32
	<i>Quasi-Steady State Approximation</i>	33
	<i>Rate-Controlled Constrained Equilibrium</i>	35
	<i>Computational Singular Perturbation</i>	36
	<i>Intrinsic Low-Dimensional Manifold</i>	37
	<i>Proper Orthogonal Decomposition</i>	39
	<i>Invariant Constrained Equilibrium Edge Pre-image Curve</i>	40
2.4	Storage/Retrieval	42
	<i>Look-Up Table</i>	42
	<i>Repro-Modelling</i>	43
	<i>Piece-Wise Reusable Implementation of Solution Mapping</i>	44
	<i>Artificial Neural Network</i>	45
	<i>In Situ Adaptive Tabulation</i>	46
2.5	The State of the Art	50
3	Modelling of Stirred Reactors	51
3.1	Fundamental Definitions	51
3.2	Gas Phase Thermochemistry	53
	<i>Equation of State for Perfect Gases</i>	53
	<i>Stoichiometry</i>	53
	<i>Reaction Mechanism</i>	54
	<i>Rate of Reaction</i>	55
	<i>Thermochemical Equilibrium</i>	56
3.3	Equations of Balance	57
3.4	Partially Stirred Reactor with IEM Model	57

3.5	Pairwise Mixing Stirred Reactor	58
3.6	The Geometry of Reactive Systems	60
	<i>Composition Space</i>	60
	<i>Mixture Temperature</i>	61
	<i>Reaction Mapping</i>	61
	<i>Reaction Vector</i>	62
	<i>Evolution Equations of PaSR/IEM</i>	63
	<i>Evolution Equations of PMSR</i>	63
4	Numerical Procedure	64
4.1	Operator Splitting Technique	64
4.2	Integration of Mixing Vector	65
	<i>IEM Mixing Model</i>	65
	<i>PMSR Mixing Model</i>	65
4.3	Integration of the Reaction Vector	66
	<i>Backward Differentiation Formula</i>	66
	<i>Truncation Error Control</i>	67
5	<i>In Situ</i> Adaptive Tabulation	69
5.1	Linearized Reaction Mapping	69
5.2	Ellipsoid of Accuracy	70
5.3	Hyper-ellipsoid Growth	72
5.4	Adaptive Tabulation Procedure	75
6	Results and Discussion	79
6.1	Code Verification	79
	<i>Numerical Integration Verification Test</i>	79
	<i>Error Control Verification Test</i>	81
6.2	Analysis of ISAT Accuracy	83
	<i>Error Metrics</i>	83
	<i>PMSR with a CO/O₂ Mixture</i>	84
	Influence of the time scale ratio	84
	Influence of the statistical process seed	90
	Influence of the ISAT error tolerance	90
	Influence of the ISAT lower bound	91
	<i>PMSR with a CH₄/Air Mixture</i>	92
6.3	Analysis of ISAT Performance	95
	<i>ISAT Performance for CO/O₂ Mixtures</i>	96
	<i>ISAT Performance for CH₄/Air Mixtures</i>	99
6.4	Analysis of ISAT Memory Usage	101
	<i>ISAT Memory Complexity</i>	101
	<i>ISAT Memory Cost for CO/O₂ Mixtures</i>	103
	<i>ISAT Memory Cost for CH₄/Air Mixtures</i>	103
7	Conclusions and Suggestions	105
7.1	Contributions of this Dissertation	105

7.2	Suggestions for Further Works	106
	Bibliography	108
A	Dimensionless Parameters	119
A.1	Dimensionless Time	119
A.2	Reduced Temperature	119
A.3	Ensemble Average of Reduced Temperature	119
A.4	Ensemble Variance of Reduced Temperature	120
B	Analysis of ISAT Efficiency	122
B.1	Necessary Condition for Efficiency	122
B.2	Empirical Metrics	122
B.3	Addition/Retrieve Relation	123
C	Conference Paper	124

List of Figures

1.1	Schematic representation of an industrial process furnace. Adapted from http://en.wikipedia.org/wiki/Furnace	24
1.2	Sketch of reverse flow combustor gas turbine. Adapted from http://en.wikipedia.org/wiki/Capstone_Turbine	25
2.1	Illustration of the classification of the different approaches. <i>S/M</i> : reduction to skeletal mechanism; <i>D/R</i> : dimension reduction; <i>S/R</i> : storage and retrieval.	29
3.1	Sketch of the composition space and its subsets.	60
3.2	Sketch of a trajectory in composition space departing from an initial composition ϕ_0 until the chemical equilibrium.	62
5.1	The region of accuracy for a constant approximation is a hyper-ellipsoid in composition space.	71
5.2	Growth process of the original hyper-ellipsoid.	73
5.3	Sketch of the binary search trees created by ISAT algorithm (leaves are black and nodes white).	76
5.4	Sketch of cutting plane in relation to EOA position.	77
5.5	Binary search tree before and after the addition of a new node.	78
5.6	A flowchart showing all step of ISAT algorithm.	78
6.1	Evolution of T and Y_{OH} for the first verification test.	81
6.2	Behavior of the ISAT global error as function of the error tolerance for the second verification test.	83
6.3	Comparison between DI and ISAT results of ensemble average of reduced temperature for cases 1 and 2.	85
6.4	Comparison between DI and ISAT results of ensemble variance of reduced temperature for cases 1 and 2.	86
6.5	Evolution of relative local error for ensemble average of the reduced temperature and of the O mass fraction for cases 1 and 2.	87
6.6	Evolution of relative local error for ensemble variance of the reduced temperature and of the O mass fraction for cases 1 and 2.	88
6.7	Comparison between DI and ISAT computations of the mean histograms (over the last 50 residence times) of the reduced temperature for cases 1 and 2.	88
6.8	Comparison between DI and ISAT computations of the mean histograms (over the last 50 residence times) of the O mass fraction for cases 1 and 2.	89
6.9	Comparison between DI and ISAT results (using different seeds) of reduced temperature ensemble average and the corresponding relative local errors for cases 1 and 2.	89
6.10	Comparison between DI and ISAT computations (using different seeds) of the mean histograms (over the last 50 residence times) of the reduced temperature for cases 1 and 2 .	90

6.11	Absolute global errors for cases 1 and 2 as function of the error tolerance, using a binary search tree with 50k entries.	91
6.12	Comparison between DI and ISAT results of the ensemble average of the reduced temperature and <i>OH</i> mass fraction for case 3.	93
6.13	Comparison between DI and ISAT results of the ensemble variance of the reduced temperature and <i>OH</i> mass fraction for case 3.	94
6.14	Evolution of relative local error of the first two statistical moments of the reduced temperature and <i>OH</i> mass fraction for case 3.	94
6.15	Comparison between DI and ISAT computations of the mean histograms (over the last 50 residence times) of the reduced temperature and <i>HCO</i> mass fraction for case 3.	95
6.16	Evolution of the ISAT algorithm outputs and of the height of ISAT binary search tree for cases 1 and 2.	96
6.17	Evolution of the rates of change of each ISAT algorithm outputs and of the height of the ISAT binary search tree for cases 1 and 2.	97
6.18	Evolution of the ISAT algorithm outputs and of the height of the ISAT binary search tree for case 3.	100
6.19	Evolution of the rates of change of each ISAT algorithm outputs and of the height of the ISAT binary search tree for case 3.	100

List of Tables

1.1	Energy supply structure by source for Brazil in 2008 and World in 2007 (EPE, 2009) [16].	23
3.1	Reaction mechanism for carbon monoxide (CO) oxidation. In this table M represent a third body with a specific efficiency for each species ($f_{O_2} = 0.4$, $f_{CO} = 0.75$ and $f_{CO_2} = 1.5$).	54
6.1	Skeletal reaction mechanism for methane/air combustion.	80
6.2	PMSR parameters used in the code verification tests.	82
6.3	Parameters used in the simulation of a CO/O_2 mixture in a PMSR.	85
6.4	Mean and maximum relative errors for cases 1 and 2, using a binary search tree with 50k entries.	86
6.5	Absolute global error as function of ε_{tol} and κ .	92
6.6	Parameters for a PMSR of CH_4/Air that behaves like a partially stirred reactor.	93
6.7	Mean and maximum relative errors for case 3, using a binary search tree with 60k entries.	95
6.8	Comparison between the computational time spent by DI and ISAT in cases 1 and 2 and the corresponding speed-up factors.	99
6.9	Comparison between the memory cost of some data types in cases 1 and 2 using two different implementations of the ISAT technique.	103
6.10	Comparison between the memory cost of some data types in case 3 using two different implementations of the ISAT technique.	104
B.1	Empirical metrics for the computational time spent at each output of ISAT algorithm and DI.	123

Nomenclature

Upper-case Roman

$\mathbf{A}(\phi, t)$	mapping gradient matrix
\mathbf{B}	scaling matrix
\mathbf{G}	rank-one modification matrix
\mathbf{I}	identity matrix
\mathbf{J}	Jacobian matrix of \mathbf{N}
\mathbf{L}'	new EOA Cholesky matrix
\mathbf{L}	EOA Cholesky matrix
\mathbf{N}	nonlinear system of algebraic equations
$\mathbf{R}(\phi, t)$	reaction mapping of ϕ
$\mathbf{R}^c(\phi, t)$	constant approximation for $\mathbf{R}(\phi, t)$
$\mathbf{R}^l(\phi, t)$	linear approximation for $\mathbf{R}(\phi, t)$
$\mathbf{S}(\phi, t)$	reaction vector
\mathbf{U}	real square orthogonal matrix
\mathbf{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
\bar{W}	mean molar mass
$\tilde{\mathbf{A}}$	modification of \mathbf{A}
$A_{ij}(\phi, t)$	components of $\mathbf{A}(\phi, t)$
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°	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
$R_i(\phi, t)$	i -th component of $\mathbf{R}(\phi, t)$
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

\mathbf{v}	cutting plane normal vector
\dot{m}	mass flow rate
\mathbf{u}	velocity field
\tilde{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°	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

$\Gamma(t)$	mixing vector
Σ	real square diagonal matrix
$\Delta\tau$	time interval
ΔH_j°	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
$\tilde{\Sigma}$	modification of Σ

Lower-case Greek

α_j	coefficients of BDF method
β_j	j -th reaction temperature exponent
ϵ	vector with the local truncation errors
$\tilde{\phi}$	transformed ϕ
ϕ	composition
ϕ_0	initial composition
ϕ_q	query composition
ϕ_{mix}	solution of the mixing system
ζ	constant vector
ζ_1	constant vector
ζ_2	constant vector
$\delta\phi$	composition displacement
$\dot{\omega}_i$	i -th chemical species reaction rate
ϵ_i	i -th component of ϵ
ϵ_G	global error of ISAT
γ	rank-one modification constant
κ	lower bound
ν''_{ij}	reverse stoichiometric coefficients

ν'_{ij}	forward stoichiometric coefficients
ν_{ij}	overall stoichiometric coefficients
$\phi_i(t_n)$	i -th component of $\boldsymbol{\phi}(t_n)$
$\tilde{\phi}_q$	Euclidean norm of $\tilde{\boldsymbol{\phi}}_q$
ψ	generic property
ρ	mixture density
ρ_i	i -th chemical species partial density
σ_i	singular values of \mathbf{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
$\tilde{\sigma}_i$	singular values of $\tilde{\mathbf{A}}$

Superscripts

*	dimensionless quantity
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

$\#(\mathbf{data})$ memory cost of \mathbf{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
ILDMM	intrinsic low-dimensional manifold
ISAT	<i>in situ</i> 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 dioxide
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* .