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THREE-DIMENSIONAL FINITE VOLUME COMPUTATION OF TiC COMBUSTION SYNTHESIS

***A. Aoufi[1] and G. Damamme[2]**

[1] PECM, UMR CNRS 5146,
Centre SMS, ENSMSE,
158 cours Fauriel,
42023 Saint-Etienne cedex 2,
France.
aoufi@emse.fr

[2] CEA-DAM/DIF,
Centre Ile de France,
BP 12,
91680 Bruyères-le-Châtel,
France.
gilles.damamme@cea.fr

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ABSTRACT

Introduction In this work, we consider titanium-carbide combustion synthesis by self-propagating high temperature synthesis process, ignited by radiative heat transfer on a part of the surface. The mathematical modelling is based on a coupling between a nonlinear parabolic equation expressing the enthalpy balance of the system - it with nonhomogeneous Neumann boundary conditions and a nonlinear differential equation describing the exothermic chemical reaction in the system. The temperature field is denoted by T and ξ is the conversion rate.

$$\frac{d\xi}{dt} = k\left(T\right)\left(1-\xi\right), \;\; \xi(.,0) = 0,$$

$$\frac{\partial H\left(T,\xi\right)}{\partial t} = \nabla.\left(\nabla\varphi\left(T\right)\right) + S\left(T,\xi\right), \qquad , -\nabla\varphi\left(T\right).n = G_{\partial\Omega}\left(T\right) = \epsilon\,\sigma\,\left(T^4 - T_{\partial\Omega}^4\right).$$

where $S\left(T,\xi\right) = Q\;k\left(T\right)\;\left(1-\xi\right)$ is the exothermic source term with Q - *heat of the reaction* -.

Error estimates of the Finite volume discretization An implicit finite volume scheme is constructed for the discretization of the governing equations of the process. For each element K of the triangulation $\mathcal{T}$ of the domain Ω, and $[t_n, t_{n+1}]$ a temporal interval, the set of discrete equations writes

$$\xi_K^{n+1} = \frac{\xi_K^n + \Delta t_n.k\left(T_K^{n+1}\right)}{1+\Delta t_n.k\left(T_K^{n+1}\right)},$$

$$m\left(K\right)\frac{H\left(T_K^{n+1},\xi_K^{n+1}\right) - H\left(T_K^n,\xi_K^n\right)}{\Delta t_n} - \sum_{L\in N_{int}(K)} W_{K,L}\;\;\left(\varphi\left(T_L^{n+1}\right) - \varphi\left(T_K^{n+1}\right)\right)$$
$$= -\sum_{L\in N_{ext}(K)} m\left(L\right)\;G_{\partial\Omega}\left(T_L^{n+1}\right) + m\left(K\right)\;S_K^{n+1}.$$

theorem 1. *Let $t_f > 0$, $D^M(\mathcal{T})$ a discretization of $\Omega \times]0, t_f[$, and $0 \leq n \leq M$. let (T, ξ) be the unique solution of the formal problem and $T_K^n = T(x_K, t_n)$, $\xi_K^n = \xi(x_K, t_n)$ for each cell $K \in \mathcal{T}$. Let $L \in N(K)$. Defining $EE_K^{n,n+1}$, $ES_K^{n,n+1}$ and $ED_K^{n,n+1}$ by the following formula*

$$
\begin{aligned}
EE_K^{n,n+1} &= \frac{H\left(T_K^{n+1}, \xi_K^{n+1}\right) - H\left(T_K^n, \xi_K^n\right)}{\Delta t_n} - \frac{1}{\Delta t_n} \frac{1}{m(K)} \int_{t_n}^{t_{n+1}} \int_K H\left(T(x,t), \xi(x,t)\right)_t \, dx \, dt, \\
ES_K^{n,n+1} &= S\left(T_K^{n+1}, \xi_K^{n+1}\right) - \frac{1}{\Delta t_n} \frac{1}{m(K)} \int_{t_n}^{t_{n+1}} \int_K S\left(T(x,t), \xi(x,t)\right) \, dx \, dt, \\
ED_{K,L}^{n,n+1} &= W_{K,L} \left(\varphi\left(T_L^{n+1}\right) - \varphi\left(T_K^{n+1}\right)\right) + \frac{1}{\Delta t_n} \frac{1}{m(K)} \int_{t_n}^{t_{n+1}} \int_{e_{KL}} \nabla\varphi\left(T(x,t)\right) . n_{KL} \, dx \, dt
\end{aligned}
$$

then the truncation error of the implicit scheme, $E_K^{n,n+1}$, with respect to cell K, defined as $E_K^{n,n+1} = EE_K^{n,n+1} + ED_{K,L}^{n,n+1} + ES_K^{n,n+1}$, is such that there exists two strictly positive constants C_1, C_2, independent of K, L and n such that

$$\left| E_K^{n,n+1} \right| \leq C_1 \, h + C_2 \, \Delta t$$

hence, the numerical scheme is first order accurate in time and space.

Performance tuning of the numerical software An important issue is the analysis of the code's behaviour on processor's memory hierarchy. Experiments using hardware performance counters are presented in order to determine the relative importance of misses/trashing rates for L_1, L_2 and TLB caches for various sizes of the three-dimensional mesh. Results of hand tuning optimization of the code are reported and discussed. A detailed performance comparison of several iterative sparse linear solvers - SOR, Stone's SIP, SI - with respect to the elapsed time and the megaflop rate is presented.

Numerical Simulation results Time-step and grid refinement study are reported. Investigation of the influence of the heat supply boundary conditions over the ignition and propagation of the combustion front in the reactive mixture is realized. Numerical simulation movies showing the ignition and propagation of the combustion synthesis front inside the material are presented.

Figure 1: *Propagation of the combustion front (left), cooling of the material (right)*

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