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Computation of chemically reacting flow on parallel systems

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The aim of this paper is to report on progress made in the development of a generally-applicable predictive procedure for chemically reacting turbulent flows in various types of axisymmetric reactors. For that purpose a code, which solves the Navier-Stokes equations for chemical reactor problems, has been developed. The main contribution here is in the assessment of a complete Reynolds-stress transport model (RSM). The RSM was compared with the results obtained by a standard $k-\epsilon$ model for the chemical reactor considered in the present study. Both models, together with the governing equations, were discretized using a co-located, finite-volume method. The coupling between the pressure and velocity equations is achieved using the SIMPLE algorithm and the resulting iterative equations are solved using either the standard Tri-Diagonal Matrix Algorithm (TDMA) or a preconditioned conjugate gradient algorithm (PCCG). A parallel version of the code was developed within the Communicating Sequential Process (CSP) programming model, implemented within a message passing harness portable to both shared- and distributed-memory systems. Parallel performances of the code are presented for the Intel i860 and IBM-SP2.

1. INTRODUCTION

It is very often the case that a high level of mixing of reactants is required within a reactor in order to ensure complete reaction. Therefore reactors need to provide the conditions for efficient mixing and this, together with the chemical kinetics, make the flow within a reactor very unstable and more turbulent when compared to non-reacting flows. This is the main motivation for introducing and testing more advanced turbulence models for the chemically reacting flows. More advanced turbulence modelling, improved chemical reaction kinetic schemes and numerically finer grids are prerequisite for better predictions of chemically reacting flows. These higher quality calculations are computationally very demanding and require large scale computational resources which will only be met through the application of parallel processing technology.

1.1. Description of problem

We are concerned with chemically reacting flows in pipe type geometries. The geometries can be modified with the inclusion of obstacles, giving a variety of reactor configurations which can be studied. The particular reaction of interest is the oxidation of titanium tetrachloride to produce pigmentary titania (TiO_2). This oxidation process involves sev-

eral complicated stages which may include the nucleation, growth and coagulation of the titania and the dissociation and recombination of chlorine product. In general the reactors have multiple inlets through which the feed materials (O_2 and $TiCl_4$) are introduced at various temperatures and velocities. The products (and any unreacted feed materials) are convected downstream and out of the reactor.

An important feature of the current numerical scheme is the way the titania pigment is modelled. Initially titania nuclei are produced which, as they proceed down the reactor, grow. The particles will also collide and may coalesce together. This process produces a continuous size distribution of titania particles. Numerically the continuous particle size domain is discretized into a number of discrete size intervals. Details of this process can be found in Hounslow et al. [1]. A schematic of the overall process with a typical reactor configuration is shown in Figure 1.

Figure 1. Typical reactor configuration and pigment formation

2. MATHEMATICAL MODEL

The conservation of the mass and momentum, for steady-state variable density flow, may be described by the equations:

$$\frac{\partial(\rho U_i)}{\partial x_i} = 0 \quad ; \quad \frac{\partial(\rho U_i U_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \rho \overline{u_i u_j} \right] \quad (1)$$

The above set of equations is not closed and in order to achieve closure, initially the standard k - ϵ model of turbulence is considered. In this model, the unknown Reynolds stresses ($\overline{u_i u_j}$) are linearly correlated to the mean rate of strain as follows:

$$-\rho \overline{u_i u_j} = \mu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \rho \delta_{ij} k \quad (2)$$

where the turbulent viscosity μ_t is given by: $\mu_t = \rho C_\mu k^2/\epsilon$. The kinetic energy of turbulence (k) and the dissipation rate of turbulent kinetic energy (ϵ) are determined from their own transport equations.

In the present study, a fast chemistry approach has been assumed where the time scale of chemistry is very small compared with the turbulence time scale (given by k/ϵ).

Consequently it is logical to expect that the reaction rate of the chemical process within the reactor would rather be mixing then chemically dominated. In such cases the accurate predictions of turbulence is essential and therefore we consider the Reynolds-stress closure as an alternative approach to the above mentioned $k-\epsilon$ model. The Reynolds stress models, which are known to be more successful in predicting the turbulent flows (e.g. flows with recirculation, swirl etc.), are based on solving the transport equations for each stress component of the following form:

$$\begin{aligned} \overbrace{U_k \frac{\partial \overline{u_i u_j}}{\partial x_k}}^{\text{convection}} = & - \overbrace{\left(\overline{u_i u_k} \frac{\partial U_j}{\partial x_k} + \overline{u_j u_k} \frac{\partial U_i}{\partial x_k} \right)}^{\text{production}} - \overbrace{\frac{\partial}{\partial x_k} \left[\overline{u_i u_j u_k} + \frac{1}{\rho} (\overline{p' u_i} \delta_{jk} + \overline{p' u_j} \delta_{ik}) - \nu \frac{\partial \overline{u_i u_j}}{\partial x_k} \right]}^{\text{diffusion}} \\ & - \underbrace{2\nu \left(\frac{\partial \overline{u_i}}{\partial x_k} \frac{\partial \overline{u_j}}{\partial x_k} \right)}_{\text{dissipation}} + \underbrace{\frac{p'}{\rho} \left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right)}_{\text{redistribution}} \end{aligned} \quad (3)$$

The above Reynolds-stress equations are not closed as the diffusion (apart from viscous diffusion), dissipation and redistribution terms need to be modelled. In the present study, the model of Speziale et al. [2] was adopted.

Chemical reactions considered here involve a simultaneous reaction of several species for which the concentration is governed by separate differential equations. The conservation equation for the mass fraction (m) of the species j can be written as:

$$\frac{\partial(\rho U_i m_j)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu_t}{Sc_t} \frac{\partial m_j}{\partial x_i} \right) + S_j \quad (4)$$

where Sc_t is an effective Schmidt number and S_j is the mass rate of creation or depletion of species j .

In order to determine the temperature field within the reactor we solve the transport equation for the mixture enthalpy (h) of the following form:

$$\frac{\partial(\rho U_i h)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\frac{k + k_t}{C_p} \left(\frac{\partial h}{\partial x_i} - \sum_j h_j \frac{\partial m_j}{\partial x_i} \right) \right] - \frac{\partial}{\partial x_i} \sum_j h_j J_{ji} - \tau_{ij} \frac{\partial U_i}{\partial x_j} + S_h \quad (5)$$

where k and k_t are molecular and effective conductivity, C_p is mixture specific heat capacity, J_{ji} corresponds to the flux of species j along direction i , τ_{ij} stands for deviatoric stress tensor and finally S_h is an enthalpy source term for chemical reactions.

Formation of solid particles is controlled by three separate processes; namely nucleation, surface growth and coagulation resulting in continuous particle size distribution at the reactor outlet. In order to numerically simulate this distribution, the continuous particle size distribution is discretized by a finite number of class sizes (minimum 12). Each class size is then treated as a separate chemical species whose concentration is governed by the differential equation of the same form as equation (4).

3. PARALLEL IMPLEMENTATION

The differential transport equations are transferred into their algebraic form using a standard finite volume technique. Co-located grid arrangement, which assumes the placement of all dependent variables at the centre of control volume, has been used.

The parallel implementation of the code has been developed using the Communicating Sequential Process (CSP) programming model. Each process runs its own code and communicates and synchronizes its actions with other processes by exchanging messages. Typically a single process is assigned to a single processor. The code can use a various type of message passing harnesses including Intel Specific (NX/2) for Intel i860 hypercube and PVM or MPI for IBM SP2 system.

The code is parallelised using a traditional domain decomposition strategy whereby the global domain is partitioned into rectangular subdomains which are allocated to unique processes. To ease the implementation of the computations a buffer of two grid points (Halo cells) is added to the rectangular domains to accommodate the finite difference and finite volume computational stencils on both real and subdomain boundaries. Figure 2 shows a general partitioning and how the buffer data is replicated around each subdomain. For the global data circulation (required for the calculation of residuals) the processors are assumed to map into a ring topology, each processor in the ring having an identifying index (Idnode), and data is circulated to processors with increasing index. The processor with the largest index circulates the data to the first processor.

Figure 2. Allocation of grid to four subdomains

The algebraic equations generated by the process of discretization are solved using a standard Tri-Diagonal Matrix Algorithm (TDMA) for all equations apart from the

pressure correction equation. For this equation the Pre-conditioned Conjugate Gradient (PCCG) Method was used. Both Solvers are well-established within the CFD community but it is still important to emphasize a couple of points concerning their parallel implementation. The parallel implementation of the TDMA solver involves limiting the range of the back-substitution step. After each sweep of the solver the halo regions are updated and it is these field values in neighbouring subdomains which are used as boundary conditions for the back-substitution. For the parallel implementation of the conjugate gradient method it is important to mention that the communication costs are dominated by global sums as the main steps in this algorithm involve vector products.

4. PARALLEL PERFORMANCE

The target here is to calculate the flow with chemical reactions, described in Section 1.1, on various type of parallel machines. This would include Intel i860 hypercube and IBM SP2. The main factor in determining the parallel performance of the code will be an efficiency coefficient defined as: $\eta = T_1/(nT_n)$ where T_1, T_n are the execution times using one and n processors respectively. The calculation of this parameter requires first obtaining the results for the single node and bearing in mind the large number of equations (23 in conjunction with $k - \epsilon$ model or 26 when the RSM is used) which need to be solved for the present problem, a size of computational grid is determined by memory of each node. Since the Intel i860 hypercube has only 16 MBytes of memory per node it is only possible to adopt 64×16 grid size for a single processor run.

Table 1 details the performance of the code using both $k - \epsilon$ and RSM models of turbulence for different processor configurations. A previous study [3] showed that for this type of geometry (very long thin pipes) the best performances are achieved when partitioning is done along the axial direction and therefore the same approach is adopted here. The timings given are in seconds per 100 iterations for an Intel i860 hypercube (64 nodes with 16 MBytes of memory per node). The total time (T_{total}) is the sum of the communication (T_{com}) times and calculation times (T_{calc}). The communication times are comprised of the times required to exchange informations between processors (T_{halo}) and of global communication times (T_{circ}).

In general both models produced a very good efficiency for the present number of processors. Results obtained by the $k - \epsilon$ model are slightly better which is probably due to the need to exchange a larger amount of data between processors when using the RSM. There is only a modest increase in total RSM computation time (compared with $k - \epsilon$ results) indicating that the present computing time is predominantly spent on calculations within the chemical model.

Table 2 gives results for the same runs but now on IBM-SP2 machine (14 thin nodes with 64 Mbytes and 2 thick nodes with 128 Mbytes of memory). The MPI message passing harness is used here for communication between processors. Results presented here are very similar in terms of efficiency compared with previous table indicating a very good

scalability of the present code.

Table 1
Total efficiency on Intel i860a

	k- ϵ model				RSM model			
	$T_{total}(s)$	$T_{calc}(s)$	$T_{com}(s)$	$\eta(\%)$	$T_{total}(s)$	$T_{calc}(s)$	$T_{com}(s)$	$\eta(\%)$
1x1	701	701	–	100	745	745	–	100
2x1	354.6	340.6	14	98.8	380.6	365.4	15.2	97.8
4x1	200	168	32	87.6	216	175	41	86.2
8x1	109	84	25	80.4	117	88	29	79.6

Table 2
Total efficiency on IBM SP2

	k- ϵ model				RSM model			
	$T_{total}(s)$	$T_{calc}(s)$	$T_{com}(s)$	$\eta(\%)$	$T_{total}(s)$	$T_{calc}(s)$	$T_{com}(s)$	$\eta(\%)$
1x1	210.2	210.2	–	100	218	218	–	100
2x1	107.2	100.5	6.7	98	113	108.6	4.4	96.4
4x1	59.5	52.6	6.9	88.3	62	54.2	7.8	87.9
8x1	33.1	27.4	5.7	79.4	34.7	28.2	6.5	78.5

5. RESULTS

This section is concerned with the results obtained for chemically reacting flows in pipe type geometries (TIOXIDE reactor). The particular reaction of interest is described in Section 1.1. Figures 3 and 4 show the contours for both reactants ($TiCl_4$ and O_2) and products (TiO_2 and Cl_2) of the main chemical reaction occurring within the reactor. The results are presented for both turbulence models. It is clear that two models lead to a different level of mixing and, therefore, the distribution of reactants and creation of the products are occurring at different positions within the reactor. For example the contours of the main product Cl_2 are more distorted along the line where the strongest mixing between the incoming horizontal jet and vertical top wall jets occur.

This difference of product and reactant concentrations within the reactor will ultimately affect the wall deposition rate as well as the size characteristics of the titania particles at the outlet. These two parameters are of critical importance since, the deposition rate would have direct effect in determining whether or not a catastrophic build-up on the wall will arise and furthermore, for any particulate product, their properties depend on the size of the individual particles created.

Temperature and $TiCl_4$ concentration profiles along reactor wall are plotted in Figures 5 and 6 respectively. Clearly, two models produce a different results so that in the case of maximum temperature point, two models differ from each other by a 100 K. Since a

Figure 3. Chemical reactor. $k-\epsilon$ results.

Figure 4. Chemical reactor. RSM results.

maximum metal temperature is a crucial design parameter, an error here can have serious impact on safety and costs.

Figure 5. Temperature distribution along the wall.

Figure 6. TiCl_4 distribution along the wall.

Two previously shown curves can be used to estimate a deposition rate on the wall using simple Arrhenius formula: deposition rate $\sim [\text{TiCl}_4] \exp(-20000/T)$. The deposition rate calculated in this way is shown in Figure 7. Two models produced a factor of 2 in the peak deposition rate which is clearly very significant.

Creation of solid particles is directly controlled by the reaction rate of each species in each particular reaction. In the present model reaction rate is chosen as minimum between

Figure 7. Wall deposition rate

Figure 8. Mass distribution of solid particle.

standard Arrhenius reaction rate and Magnussen and Hjertager model (MH, [4]). In laminar flows the reaction rate is controlled by Arrhenius model while MH model takes into account the influence of turbulence. The MH model contains an empirical constant (C) which is assumed to be $C=1$ in present study. Figure 8 includes results for mass distribution obtained by both turbulence models. Clearly, RSM model alters overall mass distribution of particles compared to the $k-\epsilon$ model.

6. CONCLUSIONS

The Reynolds-stress model of turbulence has been used to calculate the chemically reacting flow. A code has been ported on two different parallel platforms (Intel i860 and IBM-SP2) and satisfactory efficiency has been achieved. It was shown through comparison with simple $k-\epsilon$ model of turbulence that a difference in turbulence field can have an important impact on prediction of some important reactor parameters. Thus, two different approaches to turbulence modelling resulted in the difference for the peak deposition rate by a factor of two and furthermore in different particle size distributions at the reactor outlet.

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