

# Analysis of a transport equation for molar mass for steady-state simulation of reactive flow with variable, volumetric expansion

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## 1 Introduction

In this contribution, we present the work in progress on an in-depth analysis of Baudrez et al. (2007). The aim of the presented work is to give a rigorous derivation of the numerical implementation, and an analysis of the impact of varying degrees of mixture expansion on the performance of the solver, with and without the use of the molar mass equation. To make this analysis possible, a number of modifications have been made to the work presented by Baudrez et al. (2007).

Baudrez et al. (2007) use a two-phase gas–solid flow model. The drag term that couples the movement of the phases in the two-phase model is believed to have an effect on convergence. Also, the speed of sound in a gas–solid mixture is a complex function of the volume fraction of the solid phase (De Wilde et al., 2007). This has a profound effect on the discretization. In order to rule out effects of the drag term and a phase-dependent sound speed, a single-phase model is adopted in this work.

Baudrez et al. (2007) use a relatively complex 12-lump kinetic model, which has been replaced with an irreversible, first-order reaction in this work:



with a controllable rate coefficient  $k$  and stoichiometric coefficient  $n$ .

Other, minor, differences with the work of Baudrez et al. (2007) is that the heat of reaction is neglected and that the use of a preconditioner is avoided.

## 2 Governing equations

The governing equations for the flow are the Euler equations, written down as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \quad (2)$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = 0 \quad (3)$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho H u}{\partial x} = 0, \quad (4)$$

representing the conservation of mass, momentum and energy, respectively. Due to the variable composition, extra equations of the form

$$\frac{\partial \rho \omega_k}{\partial t} + \frac{\partial \rho \omega_k u}{\partial x} = \rho \dot{\omega}_k, \quad k = 1, \dots, N \quad (5)$$

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Solver	$\frac{N_{\text{flow}}}{N_{\text{reac}}}$	Number of iterations until convergence	CPU time: iteration ( $\mu\text{s}$ )	CPU time: error reduction ( $\mu\text{s}$ )
Coupled	–	20000	200	350
Decoupled	1/1	100000	100	800
Decoupled	10/1	80000	70	350
Decoupled + molar mass eq.	1/1	40000	90	300
Decoupled + molar mass eq.	10/1	20000	70	120

**Table 1:** Results for a reactive two-phase gas–solid flow model, with expansion of the mixture (Baudrez et al., 2007). The second column shows the number of iterations performed in the flow block, resp. in the reaction block, before switching to the other block. Shown are the number of iterations, the CPU time per iteration per grid cell, and the CPU time per grid cell to reduce the residue with a factor of ten.

have to be added to determine the mass fractions  $\omega_k$  of the components. The number of mass fraction equations (5) actually solved depends on whether they are solved simultaneously with the overall mass balance (2).

Because the enthalpy of all components is assumed to be equal, changes in the composition are manifested only in the molar mass of the mixture. The molar mass  $M$  affects the density  $\rho$  through the ideal gas law:

$$\rho = \frac{pM}{RT}, \quad \text{where } M = \left( \sum_{k=1}^N \frac{\omega_k}{M_k} \right)^{-1}. \quad (6)$$

A transport equation for molar mass is derived by Baudrez et al. (2007), and is written for a single-phase flow as:

$$\frac{\partial \rho M}{\partial t} + \frac{\partial \rho M u}{\partial x} = -\rho M^2 \sum_{k=1}^N \frac{\dot{\omega}_k}{M_k}. \quad (7)$$

### 3 Analysis

Two solvers are discussed by Baudrez et al. (2007): a coupled and a decoupled solver. The coupled solver solves equations (2) to (5) simultaneously. Table 1 summarizes the results given in the cited reference, obtained for a reactive two-phase gas–solid flow model. The coupled solver requires the smallest number of iterations to reach convergence. However, the CPU time per iteration is highest.

The decoupled solver solves equations (2) to (4) separately from the mass fraction equations (5). The first set of equations is called the *flow block*, while the last set of equations is called the *reaction block*. As can be seen in Table 1, the CPU time per iteration is significantly lower, but the number of iterations increases dramatically. There is no gain in total CPU time, as apparent from the last column.

A breakthrough is achieved when using the decoupled solver, with the equation for molar mass (7) added to the flow block. The required CPU time is lowered by a factor of three, compared to the coupled solver.

In this work, this will be analysed further. Due to the complex kinetic network used in Baudrez et al. (2007), it is impossible to quantify the expansion. Therefore the irreversible, first-order reaction (1) has been used instead, with a stoichiometric coefficient  $n$  that directly controls the expansion effect. The influence of  $n$  on the number of iterations and the CPU time will be investigated.

For a two-component mixture of ideal gases with reaction (1), the molar mass equation (7) can be derived in a slightly different way from Baudrez et al. (2007). The derivation clearly shows that the numerical implementation of the flow equations (2) to (4) can be made independent of

the mass fractions  $\omega_k$ , through the introduction of the molar mass  $M$  and equation (7). The advantage is that the boundary conditions and flux splitting can be developed on the reduced set of equations (2) to (4) and (7), without the mass fraction equations (5).

Analysis of the transport equations for the primitive variables  $\rho$ ,  $u$ ,  $p$  and  $M$  shows that the pressure  $p$  responds directly to the increase of the number of moles and the decrease of the molar mass. The increased pressure gives rise to a momentum increase, which in turn gives rise to a density decrease. Although it is obvious that all variables are linked to the increase of the number of moles, this analysis shows how the expansion ultimately results from it, through a sequence that starts with a pressure increase.

## 4 Conclusions

The presented work aims to give a detailed analysis of the performance and implementation of a coupled and a decoupled solver for the steady-state solution of single-phase flow with variable composition. The mixture contains two components  $A$  and  $B$ .  $A$  is converted into  $B$  via an irreversible, first-order reaction. The expansion of the mixture can be controlled via the stoichiometric coefficient  $n$ . The impact of the expansion on the convergence rate of the steady-state solution remains to be investigated. Analysis of the transport equations for the primitive variables shows that the expansion of the mixture is an indirect rather than a direct consequence of the increase in the number of moles. The direct consequence is an increase of the pressure.

## References

- Baudrez E., Heynderickx G., De Wilde J. and Marin G.B. (2007). Accounting for large density variations in the steady-state simulation of fluid catalytic cracking. In *Proceedings of MaCKiE-2. Mathematics in Chemical and Biochemical Kinetics and Engineering MACKiE-2*, Houston, USA, February 7–8, 2007
- De Wilde J., Constales D., Heynderickx G. and Marin G.B. (2007). Assessment of filtered gas–solid momentum transfer models via a linear wave propagation speed test. *International Journal of Multiphase Flow*, 33:616–637