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Numerical simulation of hydrogen dispersion behaviour in a partially open space by a stabilized balancing domain decomposition method

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ABSTRACT

The dispersion behaviour of leaking hydrogen in a partially open space is simulated numerically by a balancing domain decomposition method in this work. An analogy of the thermal convection problems is applied. The linear systems of Navier–Stokes equations and the convection diffusion equation are symmetrized by a pressure stabilized domain decomposition method. The interface problem after domain decomposition is solved by a balancing preconditioned conjugate gradient method. Numerical results are validated by comparing with the experimental data and available numerical results. The transient behaviour of hydrogen dispersion and accumulation in the partially open space is discussed; the mechanism of air influence is investigated and safe region inside this partially open space is classified.

1. Introduction

Safe storage is one of the several obstacles which must be overcome if hydrogen is to be used as a mainstream source of energy. Accompanying a more extensive usage of hydrogen, is the increased possibility of accidental release in the hydrogen infrastructure which comprises storage, bulk transportation and distribution, production and utilization. Hydrogen is highly flammable and will burn in air at a very wide range of concentrations between 4% and 75% by volume [1]; the minimum energy required to ignite hydrogen is very low (0.02 mJ, 10% of the minimum energy required to ignite gasoline vapour); as a result of this, the leakage of hydrogen in a confined space introduces the possibility of accidental ignition, which in the worst case, may result in an explosion. Moreover, hydrogen is odourless, colourless and tasteless and most human senses will not help to detect a leak; however, hydrogen can be handled safely when simple guidelines are observed and the user has an understanding of its behaviour.

It is difficult to visualize the hydrogen dispersion by experiment in case of hydrogen leaks, because of its low kinematic viscosity and high diffusibility and risk. As such, clarifying the hydrogen dispersion with numerical simulation becomes important [2,3]. On hydrogen dispersion, there are reports on the evaluation of leak flow rate [4], dispersion behaviour in residential areas [5], and the design of ventilation systems [6,7]. Inoue et al. reported the experimental data of a ventilation model [8], and by solving an analogy of the thermal convection problems using the Boussinesq approximation, Kanayama et al. reported a numerical simulation to it [2,9]. Although it is believed that Boussinesq approximation is no longer valid in buoyancy driven mixing flow when Atwood number exceeds 0.1 by some [10,11], this scheme does show its efficiency in large scale computation of hydrogen dispersion. Because of the computation complexity of high Rayleigh number in

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the modelling hydrogen dispersion, conventional numerical simulation methods suffer from low convergence speed, poor stability and robustness [12,13]. The Lagrange–Galerkin method is natural in the simulation to physical phenomena and it is demonstrated to be unconditionally stable for a wide class of problems [14–18]. Moreover, the linear systems of Navier–Stokes equations and the convection diffusion equation are symmetrized and a balancing *preconditioned conjugate gradient* (PCG) method is enabled to solve the interface problem of domain decomposition system [19].

The present study is to simulate the dispersion behaviour of hydrogen in a partially open space, by using a pressure stabilized scheme in a balancing domain decomposition system [20,21]. A variation of balancing domain decomposition is proposed and the efficiency is reported for simulation of hydrogen dispersion. Compared with the traditional fashion which is to employ some product-type methods as the iteration solver [9], the symmetry of the matrix enables computation problems with up to 30 million *degrees of freedom* (DOF) can be solved [22]. In order to validate the scheme on simulation of hydrogen dispersion behaviour, the present computation results are compared with experimental results reported by Inoue et al. [8]. The transient dispersion behaviour of hydrogen, as well as the dilution effect of air movement and several guidelines for safety in a ventilation model are discussed in this work.

The remaining sections are arranged as follows: Section 2 gives a brief description about the formulas and the balancing domain decomposition method. Section 3 describes the physical model and computational settings. Numerical results and discussions are presented in Section 4 and conclusions are drawn in Section 5.

2. Methods

2.1. Governing equations

Let $\partial\Omega$ be the boundary of a three-dimensional polyhedral domain Ω. $H^1(\Omega)$ is the first order Sobolev space and $L^2(\Omega)$ is be the space of 2nd power summable functions on Ω. Under the assumption that the flow field is incompressible, viscous and laminar, the solving of the model can be summarized as finding $(u, p) \in H^1(\Omega)^3 \times L^2(\Omega)$ such that for any$t \in (0, T)$, the following set of equations hold:

$$\begin{cases} \partial_t u + (u \cdot \nabla)\, u - \dfrac{1}{\rho}\nabla \cdot \sigma\,(u, p) = \dfrac{1}{\rho}\beta\,(C_r - C)\, g & \text{in } \Omega \times (0, T)\,, \\ \nabla \cdot u = 0 \end{cases} \tag{1}$$

where u is the velocity (m/s); p is the pressure (Pa); ρ is the density (const.) (kg/m^3); g is the gravity (m/s^2); β is the concentration expansion coefficient (-); C is the mass concentration (mass%) and C_r is the reference mass concentration; $\sigma\,(u, p)$ is the stress tensor (N/m^2) defined by

$$\begin{aligned} &\sigma_{ij}(u, p) \equiv -p\delta_{ij} + 2\mu D_{ij}(u), \\ &D_{ij}(u) \equiv \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad i, j = 1, 2, 3, \end{aligned} \tag{2}$$

with the Kronecker delta δ_{ij} and the viscosity μ (kg/ms).

An initial velocity u_0 is applied in Ω at $t = 0$. Dirichlet boundary conditions

$$u = \hat{u} \quad \text{on } \Gamma_1 \times (0, T) \tag{3}$$

and Neumann boundary conditions

$$\sum_{j=0}^{3} \sigma_{ij} n_j = 0 \quad \text{on } \partial\Omega \backslash \Gamma_1 \times (0, T) \tag{4}$$

are also applied, where $\Gamma_1 \subset \partial\Omega$ and n is the outward normal direction to $\partial\Omega$.

The governing equation of leaking hydrogen dispersion is to find $C \in H^1(\Omega)$ such that

$$\partial_t C + u \cdot \nabla C - \alpha \Delta C = S \quad \text{in } \Omega \times [0, T], \tag{5}$$

where α is the diffusion coefficient (m^2/s) and S is the source term (1/s). An initial concentration C_0 is applied in Ω at $t = 0$. Dirichlet and Neumann boundary conditions are set by

$$C = \widehat{C} \quad \text{on } \Gamma_2 \times [0, T] \tag{6}$$

and

$$\alpha \partial_n C = 0 \quad \text{on } \partial\Omega \backslash \Gamma_2 \times [0, T] \tag{7}$$

respectively, where $\Gamma_2 \subset \partial\Omega$, ∂_n is the outward normal derivate to $\partial\Omega$.