Applied Mathematics and Computation 338 (2018) 451–465

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Numerical analysis of the impact of pollutants on water vapour condensation in atmospheric air transonic flows

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A R T I C L E I N F O

Keywords:
Atmospheric air
CFD
Homogeneous condensation
Heterogeneous condensation
A convergent-divergent nozzle

A B S T R A C T

The paper presents a developed numerical tool in the form of a CFD code solving Reynolds-averaged Navier–Stokes equations for transonic flows of a compressible gas which is used to model the process of atmospheric air expansion in nozzles. The numerical model takes account of condensation of water vapour contained in atmospheric air. The paper presents results of numerical modelling of both homo- and heterogeneous condensation taking place as air expands in the nozzle and demonstrates the impact of the air relative humidity and pollutants on the condensation process.

1. Introduction

It is common knowledge that apart from gases, the Earth's atmosphere contains solid and liquid particles suspended in air and referred to as atmospheric aerosols. They may be of organic or inorganic origin. The former include bacteria, pollen or fungus spores, whereas inorganic aerosols contain – apart from water droplets and ice crystals – particles of smoke, soot, volcanic ash, dust from industrial processes, as well as sea salt crystals released into the atmosphere as waves splash against the seashore.

Atmospheric aerosols play an important part in weather-forming processes because they constitute condensation nuclei for water vapour included in the air. If the temperature is low enough, water vapour settles on them in the form of droplets or ice crystals producing clouds and precipitation. Water vapour may also condensate rapidly on the nuclei if air expansion occurs abruptly.

Considering the solid particles suspended in atmospheric air and being the potential source of nuclei of water vapour condensation, the dust of all kinds should first be taken into account. Coal fired in old and frequently badly regulated home boilers and stoves, as well as fumes from transport in big cities, are the biggest source of dust emissions. Dust is also emitted from industrial processes, with the power, chemical, mining and metallurgic industries being the main culprit.

The PM_{10} dust fraction is made up of a mixture of organic and inorganic particles suspended in air. It may also contain toxic substances. The PM_{10} dust contains particles with a diameter smaller than 10 µm and its example permissible limit for a 24-hour averaged concentration is 50 µg/m^3. Assuming that its main constituent is dust being the effect of solid fuel (coal, biomass) combustion and assuming the spherical shape of dust with an average radius of 10 µm, 1 kg of atmospheric air should contain about $5{\cdot}10^4$ particles of this kind of dust.

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https://doi.org/10.1016/j.amc.2018.06.047
0096-3003/

Another dust fraction, $PM_{2.5}$, containing particles with a diameter smaller than 2.5 μm, has an example the year-averaged concentration of 25 μg/m^3. Like in the previous case, for spherical dust particles with an average radius of 2.5 μm, it can be assumed that 1 kg of atmospheric air contains about $1\cdot10^6$ of such particles.

When it comes to non-anthropogenic aerosols, i.e., water droplets, particles of ice, salt, etc., it is estimated that close to the Earth's surface 1 kg of air contains $10^{10} \div 10^{12}$ such particles above land, whereas above oceans – about $4\cdot10^8$. Locally, however, their concentration may be by more than 100–1000 times higher, due to atmospheric phenomena for example. It is difficult to define their mean equivalent diameter, mainly due to their diverse features, instability and location. It is estimated that the mean size of those particles is much smaller compared to different kinds of dust and totals about 10–100 nm.

The impact of the above-mentioned pollutants on the process and character of condensation of water vapour contained in air under the conditions of rapid air expansion is assessed by means of a flow numerical modelling method based on the code described herein. The problem of modelling the condensing flow of moist air has been the focus of attention of numerous researchers for many years. The issue is analysed theoretically and analytically in works where analytical relations on the condensation wave and the Rankine–Hugoniot relations on the shock wave are put forward for the moist air two-phase flow [1,2]. Experimental and numerical studies have also been made in this field. The most significant are the works of Schnerr and his research team [3–6]. They focus both on the analysis of moist air internal flows [7–9] and on aerodynamic applications, such as the flow around an aircraft wing profile for example [10]. Recent works in this field concern external flows in the first place and they are related to aerodynamic issues mainly [11–13].

2. Thermodynamic description

Gases, air included, hardly ever occur in nature in the dry state. What is referred to as moist air is a mixture of dry air with water vapour or already condensed water. The mass of moist air is defined as the sum of dry air mass, m_a, and the total mass of water vapour and water, $m_{v,0}$:

$$m = m_a + m_{v,0} = m_a + m_v + m_l. \tag{1}$$

The state of moist air (moist gas) is defined by its (relative or absolute) humidity.

Absolute humidity (the moisture content) is defined as the ratio of the total mass of water vapour to the dry air mass:

$$x = \frac{m_v}{m_a}. \tag{2}$$

Relative humidity (often referred to as humidity for short) is defined as the real-to-maximum moisture content ratio, and for moderate pressure values, it is defined as the ratio of the water vapour partial pressure to saturation pressure. However, the relative humidity value is often given for integral parameters (in the computational practice – for stationary parameters at the investigated area inlet), and it is expressed in percentages. The result is then as follows:

$$\Phi_0 = \frac{p_{v,0}}{p_{v,s}(T_0)} \cdot 100\%. \tag{3}$$

Knowing the relative humidity value and the moist air pressure and total temperature, it is possible to find the absolute humidity value from the following equation:

$$x = \frac{R_a}{R_v} \frac{1}{\frac{p_0}{\Phi_0/100 \cdot p_{v,s}(T_0)} - 1}. \tag{4}$$

In addition to the moist air relative and absolute humidity values, the ratio of the water (condensate) mass to the moist air mass, referred to as the wetness mass fraction, is also defined:

$$y = \frac{m_l}{m}. \tag{5}$$

The atmospheric air wetness mass fraction reaches its maximum value upon complete condensation of the entire water vapour contained in the air:

$$y_{max} = \frac{m_{v,0}}{m}, \tag{6}$$

which is usually the case for spontaneous condensation occurring if atmospheric air expands rapidly.

The relationship between absolute humidity (moisture) and the maximum wetness mass fraction is expressed in the following way:

$$x = \frac{m_{v,0}}{m_a} = \frac{m_{v,0}}{m - m_{v,0}} = \frac{m_{v,0}/m}{1 - m_{v,0}/m} = \frac{y_{max}}{1 - y_{max}}. \tag{7}$$

In aerodynamic issues, air may with a good approximation be treated as a perfect gas because under relatively small pressures and in moderate temperatures it behaves like perfect gases.

In the case of moist air, it may with a close approximation be assumed that the temperatures of the mixture, the air and the water vapour are equal:

$$T = T_a = T_v = T_l, \tag{8}$$