SUPERCRITICAL FLUIDS IN MATGAS – FACILITIES AND RESEARCH

R. Solanas^{1,2}, J. Torres^{2,3} and L. F. Vega^{2,3}

¹Institut de Ciència de Materials de Barcelona. Consejo Superior de Investigaciones Científicas (ICMAB-CSIC), Campus UAB 08193-Bellaterra (Spain) ²MATGAS Research Center, Campus UAB 08193-Bellaterra (Spain) ³Carburos Metálicos-Air Products Group, Campus UAB 08193-Bellaterra (Spain) solanas@icmab.es

The aim of this presentation is to provide an overview of the Supercritical Fluid Laboratory facility at MatGas, with some illustrative examples of research carried out during the last years.

MATGAS 2000 AIE, known as MATGAS, is a non-profit organization, born as a joint venture between Carburos Metálicos- Air Products Group, the Spanish National Research Council (Consejo Superior de Investigaciones Científicas -CSIC) and the Autonomous University of Barcelona (Universitat Autònoma de Barcelona –UAB). MATGAS was founded to advance in the research and development of MATerials and GASes, for different applications. There are two laboratories dealing with supercritical fluids: the Supercritical Fluids lab (SCF Lab) and the Computational Modeling lab.

Regarding the experimental facilities, the SCF laboratory is equipped with reactors and autonomous equipments with capacities from 10ml to 16liters. This allows us to run experiments from laboratory to pilot plant implementations. There are six small plants and one big pilot plant. The processes can reach up to 500bar, 400°C and flows of 40kgCO₂/h, depending on the experimental conditions of work. Using these facilities a broad range of experiments have been performed, including high pressure reactions, natural products extraction and separation, crystallization of pharmaceuticals, impregnation systems and drug delivery systems, cleaning, degreases and others. These experiments have been performed under several basic research projects (funded by national and international institutions, including European projects), as well as applied research projects for pharmaceutical, food, cosmetics and other applications. Selected examples will be provided and explained here.

MATGAS also perform research in supercritical fluids from a theoretical perspective, using the facilities provided in the Computational Modeling Lab. Research in this area includes molecular-based equations of state (soft-SAFT, other theories) and molecular simulations (*Ab-initio*, Monte Carlo and Molecular Dynamics). These simulations aid to understand the molecular mechanisms of the phenomena happening at high pressure and supercritical conditions, helping in the optimization of processes and materials.

