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近红外光谱分析技术预测煤质挥发分含量模型的研究

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摘　要: 应用近红外光谱方法进行煤质在线分析工作的研究, 主要进行煤中挥发分的测定。在阅读了多个光谱图的基础上, 采用多元回归方法对数据进行了分析和处理, 建立了多元线性模型, 该模型得出的煤中挥发分的预测值与人工化验标准值之间的相关系数为 0.96, 所建模型的定标标准差为 1.41。

关　键　词: 近红外光谱; 煤质; 在线监测; 挥发分

中图分类号: TQ536; TM930.12　　文献标识码: A

1　煤质在线分析的必要性和迫切性

火电厂燃煤煤质多变, 如果调整不及时, 就会严重影响电厂的安全经济运行。其中燃煤挥发分是锅炉燃烧的一个最主要的参考指标。当燃煤煤质挥发分、发热量高时, 可能造成结渣并导致喷口被烧坏; 当煤质挥发分低、灰分高时, 则可能造成灭火打炮。若能及时提供入炉煤挥发分测定结果, 锅炉运行人员据此进行相应的调整, 对保证锅炉的安全稳定运行具有很重要的意义。

传统的煤质分析均采用人工采样制样, 再对样品进行实验室仪器分析, 此过程分析速度慢, 一批煤样的分析周期约为 6～8 h, 大多数电厂当天的煤样第二天才能出报告, 远远不能满足锅炉燃烧调整、事故分析的需要。由于测试手段的限制, 使得实际需要与测试数据报出时间滞后的矛盾越来越突出, 因此, 研究如何实现煤质的快速在线监测非常必要, 本文着重于煤中挥发分测定模型的建立。

2　近红外光谱方法对煤质在线分析的原理

近红外是指波长在 780～2 500 nm 范围内的光线, 当近红外线照射到要分析的物体上时, 由于组成物体的化学键的不同, 会产生某些特征波长的吸收, 吸收度的多少与成分含量的大小有密切关系, 由于固体对近红外波长的吸收较弱, 因此适用于漫反射技术, 根据其漫反射光谱可以分析物体成分。近红外光谱分析具有以下特点:

(1) 可在非破坏(无需采制样)和非接触的条件下进行分析;

(2) 对许多煤质参数(空气干燥基水分、水分、灰分、挥发分、发热量等)可同时进行分析;

(3) 分析响应迅速;

(4) 安全性能好;

(5) 抗干扰能力强;

(6) 因为在近红外区域有很明显的 C－H 键特征吸收带, 所以近红外测定挥发分从理论上是可行的。

多年来, 国内许多光谱试验室对近红外光谱仪器的开发应用做了大量的工作, 成功地将近红外分析技术应用到了农产品、石油产品以及医学领域等方面, 本文作者是探索该技术应用于煤质挥发分在线分析的可行性, 并对某些标准煤样的近红外线光谱进行了阅读分析, 期望从煤样的漫反射光谱上, 得到煤的特征吸收波长, 通过对煤特征波长的吸光度分析得到煤质挥发分分析结果。

3　采用近红外光谱方法测定煤中挥发分

煤的工业分析是实验室煤质分析化验的主要内容, 它包括挥发分产率、水分、灰分和固定碳 4 个项目, 用做评价煤质的基本依据。根据煤的挥发分产率可以了解煤中有机质的性质, 挥发分产率又是煤分类的主要指标, 根据它可以大致判断煤的煤化程度, 所以在线测定煤中挥发分成为煤质在线监测的重中之重。

挥发分不是煤中的固有物质, 它是煤在特定条

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件下受热分解的产物。挥发分的常规测定是一项规范性很强的试验，其测定结果完全取决于规定的试验条件，例如，加热温度和加热时间，单是完成对分析煤样挥发分的测定就需要 3 h，无法满足锅炉燃烧调整的需要。曹长武等人曾提出[7]：由于煤的着火温度和挥发分之间存在良好的相关性，可以对煤粉样的着火点进行测定，据此转换成挥发分含量。如果可行，这也不失为一种适当降低测试精度而大幅度提高测试速度的好办法。

目前国内外可以实现挥发分在线测量的方法和仪器尚无报道，这是一个不容忽视的问题。因为近红外光谱分析方法对含 C－H 的有机物比较敏感，所以从理论上讲，近红外测挥发分可行。另外，光纤技术的发展也使得在线检测成为可能。

4　典型的实验光谱图

图 1 选取了试验中 4 个无水煤样的原始光谱图，图 2 为处理后的二次微分光谱图。这 4 个样品的挥发分含量（V_{ad}%）分别是：33.58、11.90、34.19、11.92。

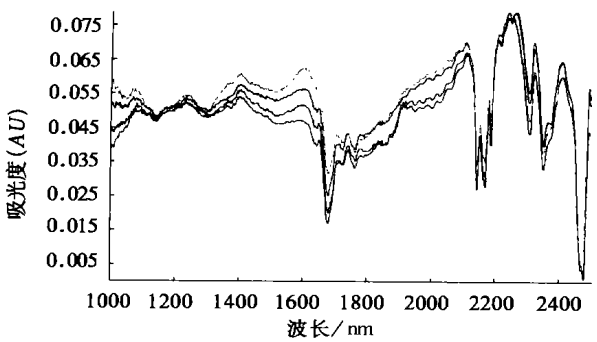

图 1　原始光谱图（基线修正后）

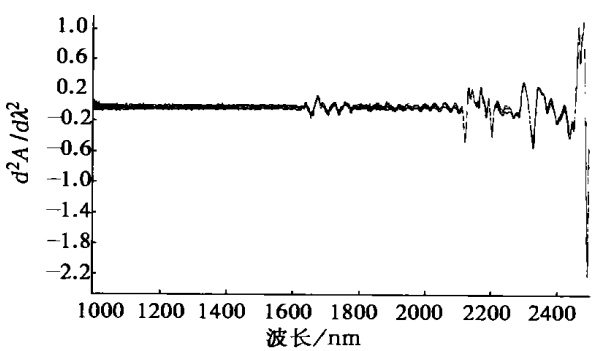

图 2　二次微分光谱图

谱图进行微分处理是为了消除光谱图基线漂移的影响，更准确地寻找顶点，但微分后噪音加强，信噪比降低。可以根据工作需要，选择原始光谱图或微分光谱图进行阅读分析。在这里，因为原始光谱图之间的相关度很好，所以我们对原始光谱图进行阅读分析。

5　数据分析与处理

选用 1 820 nm、2 100 nm、2 180 nm、2 270 nm 和 2 310 nm这几个特征吸收波长，然后从原始光谱中读取这几个波长下各样品所对应的吸光度的值。采用多元线性回归分析方法得到回归方程（读取的吸光度值与挥发分化验值之间的关系）：

挥发分预测值（%）＝ $b_0 + b_1x_1 + b_2x_2 + b_3x_3 + b_4x_4 + b_5x_5$

其中：b_0 — 常数；

b_1、b_2、b_3、b_4、b_5 — 各波长的系数；

x_1、x_2、x_3、x_4、x_5 — 各吸收波长对应的吸光度。

通过对多个样品进行回归得出系数 b_1、b_2、b_3、b_4、b_5 和常数 b_0。因为波长个数少于校正样品个数，在进行回归时，只能得到最小二乘解。

于是，回归方程为：

挥发分预测值（%）＝ $0.08 + 166.34x_1 - 656.84x_2 - 348.90x_3 + 264.64x_4 + 589.02x_5$

用上述回归方程可从未知试样的吸光度数据计算出煤中挥发分的含量。应用该回归方程得到的预测值与人工化验标准值之间的相关系数可达到0.94以上，定标标准差为 1.2。标准值与预测值属于高度相关，定标标准差偏大，值得注意的是：对于挥发分含量特别小的煤种（如挥发分含量低于 5%的无烟煤），该回归方程无效。

6　结　论

从测定煤质挥发分着手，将近红外光谱方法应用到煤质分析的研究上，本文主要介绍了挥发分的测定。采用多元线性回归方法得出回归方程，应用该回归方程得到的煤中挥发分的计算值与人工化验值之间的相关系数为 0.94，定标标准差为 1.2。挥发分大于 5%的时候，采用近红外光谱方法测定煤中挥发分应该比较有实用价值。由于近红外光谱的

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微燃烧器内甲烷催化燃烧的数值模拟

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摘 要: 联合使用 CFD 软件、FLUENT 和化学反应动力学软件 DETCHEM 对甲烷－空气混合物在有逆流换热的微燃烧器内的催化燃烧进行了数值模拟。计算中只考虑了甲烷在催化表面上的反应。燃料－空气混合物的当量比为 0.4, 燃烧器外壁面分别采用等温边界条件和与环境的对流换热边界条件, 并比较了这两种边界条件对可燃混合气燃烧的影响。计算结果表明, 催化燃烧可以实现常规方法无法实现的甲烷低温、高效转变。

关 键 词: 微燃烧器; 催化燃烧; 数值模拟
中图分类号: O643 文献标识码: A

1 引 言

随着微机电系统(MEMS)、便携式计算机、移动通讯、隐身飞行器、微小卫星、微型火箭、微型飞机、以及其它必需的移动设备等高技术的发展, 越来越迫切地需要重量轻、储能大、寿命长的新型高性能微型电源。目前, 便携式动力源基本上只能依赖于化学电池, 但是, 化学电池的单位质量储能很小。与化学电池相比, 基于燃烧的微发电系统无论在单位质量的能量储备, 还是在能量转换与利用效率上都明显地优于传统的化学电池。例如, 碳氢燃料提供的储能密度约为 40～50 MJ/kg, 而目前普遍使用的、性能最好的锂离子电池只有 0.4～0.5 MJ/kg。因此, 即使燃料的化学能只有 10%转变为电能, 碳氢燃料提供的储能密度也超过电池 10 倍以上。正是由于碳氢燃料的廉价和高储能密度的优点, 微型发电系统和微型推进系统的研究已经成为最近几年美国国防和能源高技术研究的重点投资之一。麻省理工学院、加州大学伯克利分校、普林斯顿大学以及南加州大学等分别在美国 NASA、国防部(DOD)和能源部(DOE)的支持下进行了微型火箭, 微型透平机和以燃烧方式直接发电等动力微机电系统(Power MEMS)的研究, 并取得了初步的成果。日本也把动力 MEMS 的研究列入新能源开发机构(NEDO)的研究计划之中。

基于燃烧的动力 MEMS 中, 如何实现微尺度条件下燃料的持续稳定燃烧是制约系统成败的关键因素之一。在微尺度燃烧中, 由于燃烧器尺度的减小,

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吸收受颗粒大小、颗粒密实程度等多种因素的影响, 要实现煤质的在线分析, 还有大量工作要做。

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the method under discussion is applicable for the numerical simulation of flows featuring great inverse-pressure gradients. Moreover, it can also be employed to conduct the in-depth research of various complicated three-dimensional flow phenomena in a centrifugal compressor. **Key words**: numerical simulation, q-ω turbulent flow model, high-resolution scheme, MUSCL TVD scheme, LU-SGS-GE implicit scheme

流道几何参数对低压导向器气动性能的影响＝**The Impact of Flow-passage Geometric Parameters on the Aerodynamic Performance of a Low-pressure Guide Vane Assembly** [刊, 汉] / AN Bai-tao (Institute of Engineering Thermophysics under the Chinese Academy of Sciences, Beijing, China, Post Code: 100080), WANG Shong-tao, HAN Wan-jin, WANG Zhong-qi (Harbin Institute of Technology, Harbin, China, Post Code: 150001) //Journal of Engineering for Thermal Energy & Power. — 2003, 18(6). — 572 ~ 576

By using a numerical calculation method a numerical simulation was conducted of a prototype and modified low-pressure guide vane assembly. The meridian flow passage of the latter has a relatively long casing transition section with the casing assuming a rather great outer-wall divergence angle. Gas flow is liable to separate at the outer wall, resulting in a deterioration of the cascade inlet flow of the guide vane assembly. The results of the numerical study indicate that the optimized design of the casing outer wall profile and blade contour has improved the overall aerodynamic performance of the guide vane assembly. In the case of identical calculation-domain initial conditions there is a marked reduction of outlet energy loss of the guide vane assembly. **Key words**: low-pressure guide vane assembly, numerical simulation, twisted blade, end wall profile, optimized design

CFB锅炉煤成灰特性的 6 参数模型研究＝**Six-parameter Model Study of Ash Formation Characteristics of Coals in a Circulating Fluidized Bed Boiler** [刊, 汉] / YANG Hai-rui, LU Jun-fu, XIAO Xian-bin (National Key Laboratory of Clean Coal Combustion Technology under the Tsinghua University, Beijing, China, Post Code: 100084), M. WIRSUM (Siegen University, Siegen, Germany) //Journal of Engineering for Thermal Energy & Power. — 2003, 18(6). — 577 ~ 581

An experimental method involving static combustion and cold state vibration screening is employed to study the ash formation characteristics of several Chinese coal ranks with the ash formation data-base being given for these coals. Through an analysis of the ash formation data-base of different coals it is found that the distribution of ash formation of an arbitrary narrow sieve fraction assumes a bimodal nature, i. e. being composed of relatively fine and soft ash components and relatively coarse and hard ash ones. These two kinds of ash components can simultaneously satisfy a Rosin-Rommler distribution. A six-parameter model has been set up, which can predict the ash mass portion and relevant particle size distribution of each kind of ash components. By the use of a weighting method the ash formation distribution of coal with a wide sieve fraction can be obtained. **Key words**: ash formation characteristics, soft ash, hard ash, Rosin-Rommler distribution, six-parameter model

近红外光谱分析技术预测煤质挥发分含量模型的研究＝**A Model Study Concerning the Use of Near Infrared Spectral-analysis Technology for Predicting Volatile Content of Coals** [刊, 汉] / LI Feng-rui, TANG Yu-guo (Changchun Research Institute of Optical Precision Instruments and Physics under the Chinese Academy of Sciences, Changchun, China, Post Code: 130021), XIAO Bao-lan (Department of Thermal Engineering, Jilin University, Changchun, China, Post Code: 130025) //Journal of Engineering for Thermal Energy & Power. — 2003, 18(6). — 582 ~ 583

A near infrared spectral method is used to conduct the on-line analysis of various kinds of coal with an emphasis on the determination of coal volatile content. On the basis of reading numerous spectrograms and with the use of a multiple regression method for data analysis and processing the authors have set up a multi-linear model. The correlation factor between the model-derived forecast volatile content of coal and the artificially tested standard value is found to be 0.96. The

calibration standard difference of the model is 1.41. **Key words**: near infrared spectrum, coal rank, on-line monitoring, volatile content

微燃烧器内甲烷催化燃烧的数值模拟= **Numerical Simulation of Catalytic Combustion of CH_4 in a Micro-burner** [刊, 汉] / ZHONG Bei-jing, HONG Ze-kai (Engineering Mechanics Department, Tsinghua University, Beijing, China, Post Code: 100084) // Journal of Engineering for Thermal Energy & Power. — 2003, 18(6). — 584 ~ 588

By making use of software CHD FLUENT and chemical reaction dynamics software DETCHEM a numerical simulation was conducted of the catalytic combustion of a mixture of CH_4 and air in a micro-burner featuring counter-flow heat exchange. During the calculations only the reaction of CH_4 on a catalytic surface has been taken into account. The stoichiometric ratio of fuel-air mixture is 0.4. Isothermal boundary condition and ambient convection heat-exchange boundary condition have been adopted for the burner outer wall surface. The impact of these two kinds of boundary condition on the burning of combustible fuel-air mixture was compared. Calculation results show that catalytic combustion has made it possible to realize the low-temperature and high-efficiency conversion of CH_4, which cannot be carried out by a conventional method. **Key words**: micro-burner, catalytic combustion, numerical simulation

油页岩流化床燃烧 N_2O 生成特性= **Experimental Investigation on N_2O Emission Characteristics during the Operation of an Oil Shale-fired Fluidized Bed Boiler** [刊, 汉] / DING Nai-jin, JIANG Xiu-min, WU Shao-hua (School of Energy Sources under the Harbin Institute of Technology, Harbin, China, Post Code: 150001) // Journal of Engineering for Thermal Energy & Power. — 2003, 18(6). — 589 ~ 591

On a small-sized (diameter 20mm and height 450mm) thermal-state fluidized bed combustion test rig an experimental investigation was carried out to ascertain the impact of different operating parameters on N_2O emission characteristics during the operation of a oil shale-fired fluidized bed boiler. The investigation results indicate that an increase in combustion temperature and circulation ratio, a decrease in excess air factor and the desulfurization of in-boiler limestone, etc can be conducive to decreasing N_2O generation quantity. The above finding has provided essential basic data for the design and operation of oil shale-fired circulating fluidized bed boilers. **Key words**: oil shale, N_2O, fluidized bed combustion

鼓泡式烟气脱硫原理性试验台气体流动冷模试验= **Cold Model Tests of Gas-liquid Flows in a Wet Bubbling Flue-gas Desulfurization Test Rig** [刊, 汉] / ZHONG Zhao-ping, JIN Bao-sheng, LAN Ji-xiang, et al (Education Ministry Key Laboratory of Clean Coal Power Generation and Combustion Technology under the Southeastern University, Nanjing, China, Post Code: 210096) // Journal of Engineering for Thermal Energy & Power. — 2003, 18(6). — 592 ~ 596

Cold model tests and test results are described of gas-liquid flows in a wet bubbling flue-gas desulfurization test rig. Through the tests it is found that with regard to tube-outside jets the variation of injection pipe bubbling layer height and pressure drop at a bottom seal in three kinds of test tubes is very stable. As for tube-inside jets the injector pressure drop fluctuates dramatically with the change of injection speed and insertion depth of the jet pipe, thus being regarded as very unstable. In view of the above it is recommended to employ tube-outside jets for engineering applications. Measurements were taken of the jet velocity field of jet pipe tube-outside injection at a bottom seal with the use of a PIV (particle imaging velocimetry) instrument. It was discovered that in a gas-liquid fully mixed zone the motion trajectory of the gas bubbles are very complicated with a large quantity of vortex groups being formed accompanied by an intensive perturbation of gas-liquid. When the speed is in excess of 16 m/s, the vortex groups mainly appear in the neighborhood of tube walls and the intermediate gas-liquid assumes the form of surge waves, which is very unfavorable for gas-liquid contact. **Key words**: bubbling, flue gas desulfurization, gas-liquid flow, cold model test, particle imaging velocimetry

船用汽轮机冷态启动过程中热膨胀的研究= **A Study of Thermal Expansion in the Cold-state Startup Process of a Marine Steam Turbine** [刊, 汉] / LIU Shu-yi, LI Jian-zhao (Harbin No. 703 Research Institute, Harbin, China,